



TERRASCOPE SENTINEL-2

ALGORITHM THEORETICAL BASE

DOCUMENT (ATBD)

S2 – RHOW – V120

Reference: *Terrascope Sentinel-2 Algorithm Theoretical Base Document S2 – RHOW – V120*

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LIST OF ACRONYMS

ACRONYM	EXPLANATION
ACE	Altimeter Corrected Elevations
ACIX	Atmospheric Correction Inter-comparison Exercise
AOT	Aerosol Optical Thickness
ATBD	Algorithm Theoretical Base Document
ATLAS	Atmospheric Laboratory for Applications and Science
CCI	Climate Change Initiative
CHL	Chlorophyll-a concentration
CMIX	Cloud Masking Inter-comparison Exercise
COG	Cloud-Optimized Geotiff
DEM	Digital Elevation Model
EGM96	Earth Gravitational Model 1996
ESA	European Space Agency
EURECA	European Retrieval CArrier
GeoTIFF	Geospatial Tagged Image File Format
iCOR	Image Correction for atmospheric effects
L1C	Level1C (Top-Of-Atmosphere) product
L2A	Level2A (Top-Of-Canopy) product
MEP	Mission Exploitation Platform
MSI	Multispectral Instrument
NDVI	Normalized Difference Vegetation Index
NRT	Near Real Time
OGC	Open Geospatial Consortium
PDGS	Payload Data Ground Segment
PDP	Product Distribution Portal
PROBA-V	Project for On-Board Autonomy – Vegetation
RAA	Relative Azimuth Angle
RD	Related Document
RHOW	Water-leaving reflectance
S2	Sentinel-2
SAA	Sun Azimuth Angle
SAR	Synthetic Aperture Radar
Sen2Cor	Sentinel-2 Correction
SNAP	Sentinel Application Platform
SOLSPEC	SOLar SPECTrum
SPM	Suspended Particulate Matter
SPOT	Satellite Pour l'Observation de la Terre
SRF	Spectral Response Function
SRTM	Shuttle Radar Topography Mission
SWIR	Short-Wave infrared
SZA	Solar Zenith Angle
TOA	Top-Of-Atmosphere
TOC	Top-Of-Canopy
TUR	Turbidity
UTM	Universal Transverse Mercator

Terrascope Sentinel-2

List of acronyms



VAA	View Azimuth Angle
VITO	Flemish Institute for Technological Research
VNIR	Visible and Near InfraRed
VZA	Viewing Zenith Angle
WGS84	World Geodetic System 1984
WVP	Water Vapour
XML	Extensible Markup Language

1. Introduction

1.1. Terrascope explained

Terrascope is the Belgian platform for Copernicus, PROBA-V, and SPOT-VEGETATION satellite data, products, and services. It provides easy, full, free and open access to all users without restrictions. This allows non-specialist users to explore the wealth of remote sensing information and build value-added products and services.

The following data are included:

- The SPOT-VEGETATION archive
- The PROBA-V archive
- Sentinel-1 SAR data over Belgium and its surroundings
- Sentinel-2 optical data over Europe and soon to be expanded to Africa
- Sentinel-3 optical and thermal Synergy (SYN) – Vegetation (VGT) data
- Sentinel-5P atmospheric composition data

For Sentinel-2, land surface reflectance products are obtained from the European Space Agency (ESA). Water reflectance products, on the other hand, are produced within Terrascope and the methodology is described in this ATBD.

A standard set of water quality products [Turbidity (TUR), Suspended Particle Matter (SPM), and Chlorophyll-a concentration (CHL)] derived from Sentinel-2 observations is provided in addition to the water-leaving reflectance (RHOW) products. This document explains the methodology and data content of the RHOW product.

Users have the possibility to build derived information products to their own specification, using the Terrascope processing cluster through provided virtual machines or Notebooks. This eliminates the need for data download (and consequential storage costs), because the cluster holds all of the data and it is directly accessible. Integration of data or products in your own application is facilitated through Open Geospatial Consortium (OGC) web services.

Terrascope is user centered, so any suggestions for new or enhanced functionality are welcome. Feel free to contact us: info@terrascope.be .

1.2. Scope of Document

This ATBD (Algorithm Theoretical Base Document) describes the origin and generation of the Sentinel-2 (S2) Level-2 (L2) Water-Leaving Reflectance (RHOW) data product embedded in the Terrascope Sentinel-2 Water V120 processing chain.

The document is organised as follows:

- Section 2 provides an overview of the input data needed for the processing workflow, including a description of the S2 Level-1C (L1C) input and ancillary data.
- Section 3 explains the data available to users.
- Section 4 provides a detailed description of the different processing algorithms.
- Section 5 discusses the implemented algorithm’s limitations.
- Section 6 justifies the overall workflow with a quality assessment.

1.3. Description

The S2 RHOW product is a geometrically and atmospherically corrected version of the original Copernicus L1C data with additional information on pixel classification, Aerosol Optical Thickness (AOT), and angle information: Solar Zenith Angle (SZA), Viewing Zenith Angle (VZA), and Relative Azimuth Angle (RAA).

The workflow starts from S2 L1C data as provided by ESA (Gatti et al., 2018), which is Top-Of-Atmosphere (TOA) reflectance in cartographic geometry [i.e., combined Universal Transverse Mercator (UTM) projection and World Geodetic System 1984 (WGS84) ellipsoid]. The IdePix pixel identification tool [RD3] generates a pixel identification layer which is a multiband GeoTIFF containing information about among others different types of clouds, shadows, brightness, land, and more. In parallel, iCOR (De Keukelaere et al., 2018) corrects for atmospheric effects. The output of this workflow encompasses RHOW reflectance for each spectral band, a pixel identification layer, the AOT, SZA, VZA, and RAA output layers.

This document applies to the Terrascope S2-Water V120 processing chain. Table 1.1 summarizes the main characteristics of the different Terrascope versions until V120. Table 1.2 summarizes the differences between Terrascope S2-Land [RD4] and Terrascope S2-Water.

Table 1.1: Summary of main characteristics of different Terrascope versions until V120.

Version	Main characteristics
V100	Input: L1C data Atmospheric correction: iCOR 3.0 Scene classification: IdePix v8.0.0 Output: RHOW, pixel classification, AOT, SVA, VZA, RAA
V110 & V120	Input: L1C data (adjusted base processing ESA, changes described in [RD1]) Atmospheric correction: iCOR 3.0 Scene classification: IdePix v8.0.2

Version	Main characteristics
	Output: RHOW, pixel classification, AOT, SVA, VZA, RAA (between V110 & V120 only the water quality product CHL changed)

Table 1.2: Summary of the differences between the Terrascope S2 Land and Terrascope S2-Water L2 products.

	Terrascope S2-land	Terrascope S2-water
Scene classification	Sen2Cor v2.5.5	IdePix v8.0.2
Atmospheric correction	Sen2COR v2.5.5	iCOR v3.0
Output products	Top-Of-Canopy (TOC) products	Water-Leaving Reflectance (RHOW) products

1.4. Feature added value/use case

The impact of atmospheric absorption and scattering on the TOA reflectance differs for each spectral band. In data assessment studies (e.g. band ratios, time series analysis or quantitative studies), atmospheric disturbances will hamper a good analysis. Terrascope provides a solution for users that want to work with atmospherically corrected Sentinel-2 data for water applications by making RHOW products available in Cloud-Optimized GeoTIFF (COG) format. The RHOW products are accompanied by pixel classification layers and AOT, SZA, VZA, and RAA information. These latter layers are useful for quality control or to derive new value-added products.

1.5. Related documents

Table 1.3 lists the related documents (RD) that are complementary to this ATBD. Other Reference Documents (ORD) are listed in Section 7.

Table 1.3: List of related documents.

[RD1]	Gatti, A., Galoppo, A. Castellani, C., Carriero, F. (2021). Sentinel-2 Products Specification Document, REF: S2-PDGS-TAS-DI-PSD issue 14.9. https://sentinels.copernicus.eu/documents/247904/4756619/S2-PDGS-TAS-DI-PSD-V14.9.pdf/3d3b6c9c-4334-dcc4-3aa7-f7c0deffba7
[RD2]	De Keukelaere, L., Sterckx, S., Adriaensen, S., Knaeps, E., Reusen, I., Giardino, C., ... & Vaiciute, D. (2018). Atmospheric correction of Landsat-8/OLI and Sentinel-2/MSI data using iCOR algorithm: validation for coastal and inland waters. <i>European Journal of Remote Sensing</i> , 51(1), 525-542.

	https://doi.org/10.1080/22797254.2018.1457937
[RD3]	Jan Wevers, Dagmar Müller, Jorrit Scholze, Grit Kirches, Ralf Quast, & Carsten Brockmann. (2021). IdePix for Sentinel-2 MSI Algorithm Theoretical Basis Document (Version 1.0). Zenodo. https://doi.org/10.5281/zenodo.5788067
[RD4]	De Keukelaere, L., Van De Kerchove, R., Swinnen, E., Wolters, E., Clarijs, D., Everaerts, J. (2020). Terrascope Sentinel-2 Algorithm Theoretical Base Document (ATBD) S2-TOC-V200. https://docs.terrascope.be/DataProducts/Sentinel-2/references/S2_L2A_ATBD_V200.pdf

2. Input data

2.1. General

The Terrascope processing starts from the S2 L1C data products that can be freely downloaded from the Copernicus Open Access Hub (<https://scihub.copernicus.eu/dhus/#/home>). The data are distributed in granules, also called tiles, which are 100 × 100 km² ortho-images in UTM/WGS84 projection with an overlap of 9.8 km between tiles. The tiling grid can be downloaded from [Sentinel-2 tiling grid.kml](#). The L1C data are TOA reflectance, projected in UTM zones of the WGS84 ellipsoid.

S2 L1C data are distributed by ESA as SAFE files, which includes image data in JPEG2000 format, quality indicators, auxiliary data, and metadata. The Multispectral Instrument (MSI) on-board S2 measures the Earth's reflected solar irradiance in 13 spectral bands from the Visible and Near Infra-Red (VNIR) to the Short Wave Infra-Red (SWIR), see Figure 2.1:

- 4 bands at 10 m spatial resolution: blue (492 nm centre wavelength), green (560 nm), red (665 nm) and near-infrared (833 nm).
- 6 bands at 20 m spatial resolution: 4 narrow bands for vegetation characterization (704 nm, 740 nm, 781 nm and 865 nm) and 2 larger SWIR bands (1612 nm and 2194 nm) for applications such as snow/ice/cloud detection or vegetation moisture stress assessment.
- 3 bands at 60 m spatial resolution, mainly for cloud screening and atmospheric corrections (443 nm for aerosols, 945 nm for water vapor and 1375 nm for cirrus detection).

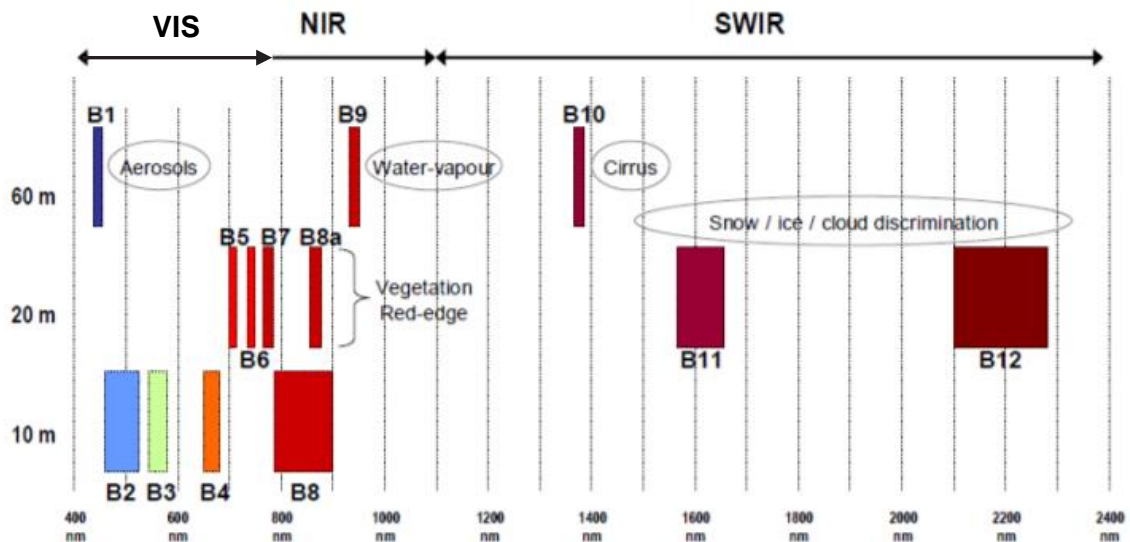


Figure 2.1: S2 MSI Spectral-Bands versus Spatial Resolution Reference [RD2].

More information on the S2 data products and tiling strategy is available on <https://sentinel.esa.int/web/sentinel/missions/sentinel-2/data-products>. Detailed information on the S2 L1C data products can be found in [RD1].

2.2. Ancillary data and models

2.2.1. Pixel classification

Pixel classification in the Terrascope S2 water workflow is performed using the IdePix v8.0.2 [RD3] Sentinel Application Platform (SNAP) plugin. The IdePix tool uses the Global Earth Topography And Sea Surface Elevation at 30 arc second (~1 km) resolution (GETASSE30) as auxiliary data. This DEM, displayed in Figure 2.2, has a global coverage and is a composite of four other DEM datasets: Shuttle Radar Topography Mission 30 (SRTM30), Altimeter Corrected Elevations (ACE), Mean Sea Surface (MSS) and the Earth Gravitational Model 1996 (EGM96). The resulting GETASSE30 dataset represents the earth topography and sea surface elevation with respect to the WGS84 ellipsoid at ~1 km resolution.

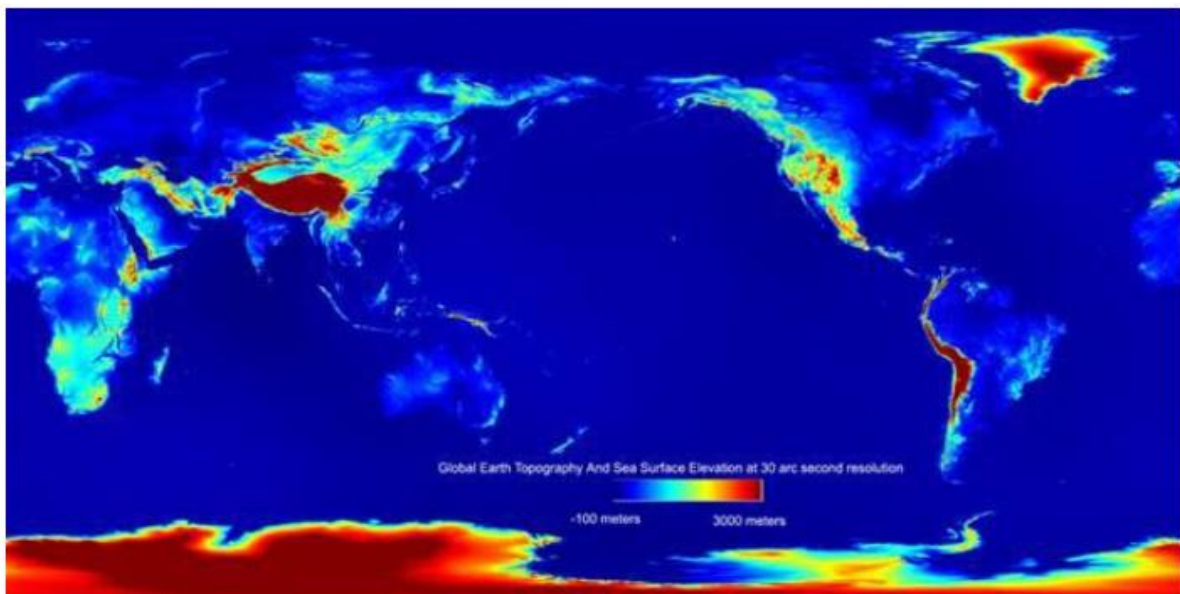


Figure 2.2: GETASSE30 DEM.

More information on the implementation is given in Section 4.1.

2.2.2. Atmospheric Correction

The atmospheric correction algorithm makes use of following algorithms, models, and ancillary data:

- **Image correction for atmospheric effects (iCOR)**
The Terrascope S2 water workflow uses iCOR [RD2] to perform the atmospheric correction. iCOR relies on the Moderate Resolution Atmospheric Transmission Model-5 (MODTRAN5, Berk et al. 2006) for the radiative transfer modelling. The iCOR implementation is described in detail in Section 4.2.
- **MODTRAN5 Look-Up-Tables (LUT)**
iCOR relies on pre-calculated Lookup Tables (LUTs) based on MODTRAN5 radiative transfer modelling. These LUTs provide atmospheric correction parameters and diffuse transmissions in function of VZA, SZA, RAA, AOT, and elevation. The parameters used to generate this LUT are explained in ANNEX I – MODTRAN5 LUT input parameters.
- **Digital Elevation Model (DEM)**
The Global Land One-km Base Elevation (GLOBE) is an 30-arc-second (~1 km) gridded, quality-controlled global DEM. The data is projected in Lat/Lon WGS84 at 0.008333° or +/- 1 km (Hastings et al., 1999). It is visualized in Figure 2.3.

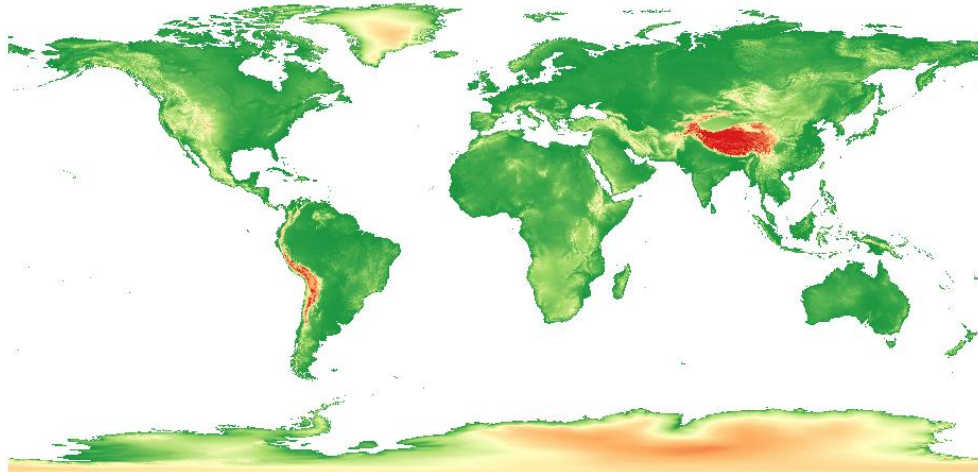


Figure 2.3: GLOBE DEM (Hastings et al., 1999).

- **Angle information**
The angle information, i.e. SZA, VZA, and RAA are obtained from the S2 L1C metadata.
- **Solar Irradiance**
The solar spectral irradiance dataset from Thuillier et al. (2003) is used in the Terrascope atmospheric correction. This dataset covers a spectral range from 200 to 2400 nm, measured

by the SOLar SPECTrum (SOLSPEC) spectrometer from the Atmospheric Laboratory for Applications and Science (ATLAS) and European Retrieval Carrier (EURECA) missions.

- **Spectral response functions (SRFs)**

The Terrascope workflow relies on the S2 SRF v3.0, released by ESA on 19/12/2017. Compared to the previous version (v2.0), this version includes updated S2A spectral responses, mainly modifying the responses for bands B01 and B02 (ESA, 2017).

- **AOT fall-back datasets**

An AOT fall-back mechanism is implemented in case the image doesn't succeed in an accurate AOT retrieval (see Section 4.2.2 Implementation). This fall-back mechanism relies on external AOT data from the Copernicus Atmospheric Monitoring Service (CAMS):

- Near-Real Time (NRT) AOT values at 550 nm - <http://apps.ecmwf.int/datasets/data/cams-nrealtime/levtype=sfc/> (Morcrette et al, 2009)
- Climatological monthly AOT averages at 550 nm (Inness et al., 2019)

3. Product data content

3.1. Product layers

3.1.1. Product data

The S2 RHOW products generated and distributed by Terrascope include several files which are the output of the iCOR processor for atmospheric correction and IdePix scene classification. Each output file in the RHOW product is formatted as a single layer compressed Cloud-Optimized GeoTIFF file. Figure 3.1 shows the S2 RHOW product file list.

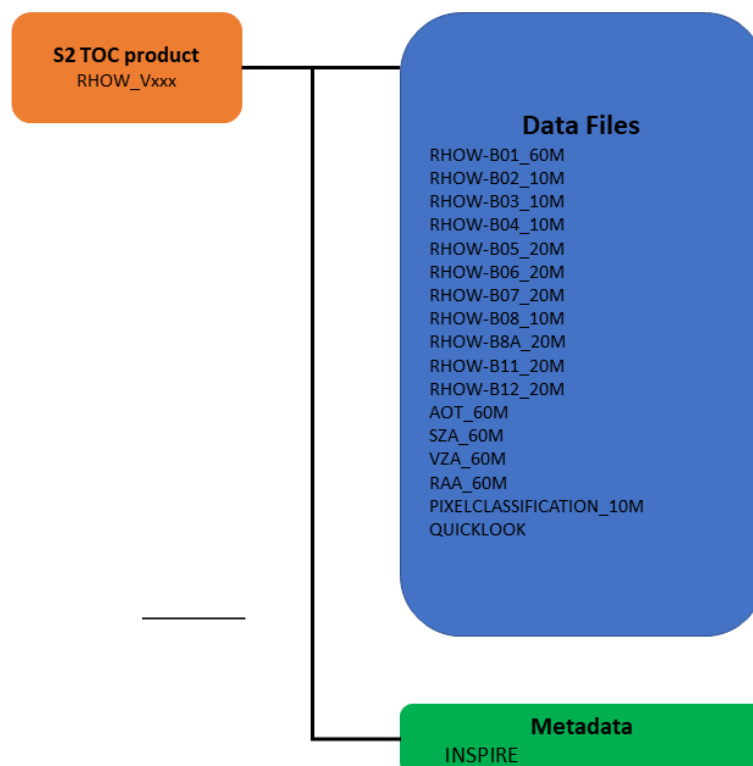


Figure 3.1: S2 RHOW product file list.

The S2 RHOW spectral bands span from the Visible and Near-Infrared (VNIR) through Shortwave Infrared (SWIR) at different spatial resolutions. The spatial and spectral characteristics are listed in Table 3.1. Note that B09 and B10 are not delivered, as these contain the water vapor and cirrus bands, respectively.

Table 3.1: Spatial and spectral characteristics of the S2 RHOW products.

Layer	Spatial resolution [m]	S2 A		S2 B	
		Central wavelength [nm]	Bandwidth [nm]	Central wavelength [nm]	Bandwidth [nm]
<i>RHOW-B01_60M</i>	60	442.7	21	442.2	21
<i>RHOW-B02_10M</i>	10	492.4	66	492.1	66
<i>RHOW-B03_10M</i>	10	559.8	36	559.0	36
<i>RHOW-B04_10M</i>	10	664.6	31	664.9	31
<i>RHOW-B05_20M</i>	20	704.5	15	703.8	16
<i>RHOW-B06_20M</i>	20	740.5	15	739.1	15
<i>RHOW-B07_20M</i>	20	782.8	20	779.7	20
<i>RHOW-B08_10M</i>	10	832.8	106	832.9	106
<i>RHOW-B8A_20M</i>	20	864.7	21	864.0	22
<i>RHOW-B11_20M</i>	20	1613.7	91	1610.4	94
<i>RHOW-B12_20M</i>	20	2202.4	175	2185.7	185

The AOT, SZA, VZA, and RAA are provided at the native 60 m resolution.

3.1.2. Product metadata

The physical pixel values in the S2 RHOW files are converted from floating point values into integers, mainly to reduce the file sizes. Table 3.2 lists the technical information of the S2 RHOW product, with information necessary to calculate the Physical Values (PV) from the Digital Numbers (DN) available in the files. This can be done using the following formula:

$$PV = DN * scaling + offset$$

Table 3.2: Characteristics of the S2 RHOW, AOT, WVP, SZA, VZA and RAA images and rescaling information. Physical min and max are the physical range that is retained in the output, the Digital Numbers (DN) are the value of the physical min and max after rescaling to integers. The slope and offset are the coefficients to use to recompute the physical values from the output files using the above equation.

	RHOW [-]	AOT [-]	SZA [°]	VZA [°]	RAA [°]
Physical min	-1.0	0.00	0	0	0
Physical max	2.0	2.5	80	12	180
DN min	-10000	0	0	0	0
DN max	20000	2500	8000	1200	18000
Scaling	0.0001	0.001	0.01	0.01	0.01
Offset	0.0	0.0	0.0	0.0	0.0

While the theoretical range of the water-leaving reflectance is [0, 1], the limits are set to -1 and 2 respectively, as slightly negative values are possible for dark areas like water surfaces, and values just exceeding 1 are possible for very bright features like clouds.

The output of the IdePix classification module provides a multiband at 10 m spatial resolution. Table 3.3 lists the different bands available in the Pixel Identification multiband file.

Table 3.3: Different bands of the Pixel Identification multiband file.

FILE	LAYER_ID	LAYER
PIXEL IDENTIFICATION	1	IDEPIX_INVALID
	2	IDEPIX_CLOUD
	3	IDEPIX_CLOUD_AMBIGUOUS
	4	IDEPIX_CLOUD_SURE
	5	IDEPIX_CLOUD_BUFFER
	6	IDEPIX_CLOUD_SHADOW
	7	IDEPIX_SNOW_ICE
	8	IDEPIX_BRIGHT
	9	IDEPIX_WHITE
	10	IDEPIX_COASTLINE
	11	IDEPIX_LAND
	12	IDEPIX_CIRRUS_SURE
	13	IDEPIX_CIRRUS_AMBIGUOUS
	14	IDEPIX_CLEAR_LAND
	15	IDEPIX_CLEAR_WATER
	16	IDEPIX_WATER
	17	IDEPIX_BRIGHTWHITE
	18	IDEPIX_VEG_RISK

19	IDEPIX_MOUNTAIN_SHADOW
20	IDEPIX_POTENTIAL_SHADOW
21	IDEPIX_CLUSTERED_CLOUD_SHADOW

In the Terrascope Virtual Machine environment, the RHOW product data can be found in `/data/MTDA/TERRASCOPE_Sentinel2/<Product_version>/<Year>/<Month>/<Day>/<Tile_ID>`

The folder structure used on the Terrascope platform is:

1. Product and version - *e.g. RHOW_V1*
2. Year – *e.g. 2021*
3. Month – *e.g. 04 for April*
4. Day – *e.g. 04*
5. Tile_ID – *e.g. S2B_20190504T105629_31UDS_RHOW_V120*

It sometimes happens that some Sentinel-2 input data are delivered multiple times when there is a switching between the receiving stations. For example, let's take the following Sentinel-2 Level-1C products:

- a) `S2B_MSIL1C_20170829T105019_N0205_R051_T31UFS_20170829T105021.zip`
- b) `S2B_MSIL1C_20170829T105019_N0205_R051_T31UFS_20170829T105633.zip`

Based on the processing timestamp in the filename (highlighted in bold), one can differentiate between redelivered products. Both products need to be stitched (mosaicked) in order to become a fully filled tile. This creates a Sentinel-2 mosaic product with the same file naming conventions as Sentinel-2 Level-1C products (see <https://sentinel.esa.int/web/sentinel/user-guides/sentinel-2-msi/naming-convention>), but with the processing timestamp always set to `19700101T000000`, e.g. `"S2B_MSIL1C_20170829T105019_N0205_R051_T31UFS_19700101T000000.zip"`

3.2. Product version

Terrascope products are produced in a controlled way. Every product has a version indicator, consistent with the Semantic Versioning 2.0.0 protocols (<https://semver.org/>). The version indicator has three digits: XYZ.

- X is 0 during prototyping and pre-operational use. X is 1 for the first operational setup, and increments when results are no longer backward compatible (i.e. any further processing will have to be adapted to deal with e.g. format changes, value scaling, etc.).
- Y is reset to 0 with an X increment. Y increments when functionality is added, but backward compatibility is guaranteed (e.g. when a different approach is taken for atmospheric or geometric correction).
- Z is reset to 0 when Y increments. Z increments when the software is patched (bug fixed) without any functional changes.

The current Terrascope Sentinel-2 water workflow version is V120.

Whenever X or Y changes, the impact of the updates will be reported and the new and previous versions of the workflow will be run in parallel for a 3-4 month period. This allows users to implement changes to their subsequent processing. Users are informed about version changes through the Terrascope newsletter (to subscribe: <https://terrascope.be/en/stay-informed>).

3.3. Product data access

The Terrascope S2 data products can be accessed through:

- Web services: Web Map Service (WMS) and Web Map Tile Service (WMTS):
https://bit.ly/TerrascopeFAQ_WMTS
Protocols for downloading images and integrating them into GIS software
- Notebooks (login required): <https://notebooks.terrascope.be/hub/login>
Programming environment to quickly access and edit data
- Virtual Machines (VM) (login required): <https://forum.terrascope.be/en/request-vm>
External computer used to view data and process it in the cloud
- OpenEO API (login required): <https://openeo.org/documentation/1.0/python/>
Python API to automate satellite data processing in the cloud

The details of each of these access points are described on <https://terrascope.be/en/services>.

4. Methodology

4.1. Pixel identification

4.1.1. Justification

Including a pixel classification in the output facilitates the exploitation of the RHOW products in further processing steps. A couple of well-known tools exists, including Sen2Cor (Mueller-Wilm et al, 2018), Fmask (Zhu et al., 2015) and IdePix [RD3]. While Terrascope-Land makes use of Sen2Cor, IdePix has been selected for TERRASCOPE water. The results of the recently organized Cloud Masking Intercomparison Exercise ([CMIX](#)) were considered to make this decision.

IdePix is also integrated in the Copernicus Climate Change Service (C3S), ESA Climate Change Initiatives (CCI) (Ocean Colour, Land Cover, Fire, Sea Surface Temperature, Water Vapour), Copernicus Global Land Service (CGLS), CODE-DE, CyanoAlert, DataCube Service for Copernicus (DCS4COP), GlobWetland Africa, Multiply, and the Sentinel-3 Mission Performance Centre (S3-MPC).

4.1.2. Implementation

IdePix is a multi-sensor pixel identification tool available as a [SNAP](#) plugin. It provides pixel identification algorithms for a wide variety of sensors like Sentinel-2, Sentinel-3, Medium Resolution Imaging Spectroradiometer (MERIS), Landsat-8, Moderate Resolution Imaging Spectroradiometer (MODIS), and the Visible Infrared Imaging Radiometer Suite (VIIRS) In contrast to many other pixel identification tools, IdePix provides non-exclusive property flags. This means a single pixel can have multiple properties, like land and cloud (semi-transparent cloud over land), land and snow (land covered with snow), or land, snow and cloud (semi-transparent cloud over snow-covered land). It provides a flags band with which all further algorithms can be triggered individually, following valid pixel expressions specified for the respective application.

In Terrascope S2 water, the SNAP IdePix plugin v8.0.2 is used. The IdePix output is a classification layer with classes as defined in Table 3.3.

4.1.3. Outlook

Future IdePix updates will be evaluated. If the updated version results in a significant improvement, the Terrascope workflow will be updated accordingly to include the new version.

4.2. Atmospheric correction

4.2.1. Justification

When electromagnetic radiation passes through the atmosphere it may be transmitted, scattered or absorbed. Using S2 data for quantitative remote sensing of land or water surfaces requires the removal of atmospheric effects, which is essential to convert radiance measured by the sensors to surface reflectance. The atmospheric effect on the radiance received by a remote sensor is significantly larger over water bodies, because water strongly absorbs the sunlight and contributes to 20 % or less of the total at-sensor radiance (e.g. Hovis and Leung, 1997). Correcting for these atmospheric effects is an essential prerequisite to retrieve accurate estimates of water-leaving reflectance, which is the basis for deriving quantitative estimates of biophysical parameters, such as CHL, TUR or SPM (Moses et al., 2017).

Terrascope S2-Water uses iCOR v3.0 [RD2] as atmospheric correction algorithm. iCOR is a scene-generic atmospheric correction tool: it works on both land and water targets (coastal, transitional, and inland waters). The tool identifies whether a pixel is water or land and applies a dedicated correction. In contrast to land surface atmospheric correction algorithms, which often assume a Lambertian surface, iCOR takes the specular reflection of the air-water interface into account (Geo et al., 2009) and corrects for adjacency effects (Sterckx et al., 2015). iCOR participated in the ACIX-I (Doxani et al., 2018) and ACIX-II atmospheric correction intercomparison exercise, jointly organized by ESA and the National Aeronautics and Space Administration (NASA). The decision on including iCOR for water was made based on the results of ACIX-Aqua (Pahlevan et al., 2021), see Section 6. iCOR is available for the user community as a plugin in the SNAP toolbox for Landsat-8, Sentinel-2, and Sentinel-3: <https://remotesensing.vito.be/case/icor>.

4.2.2. Implementation

Figure 4.1 shows the flowchart of the atmospheric correction implemented in Terrascope. Starting from S2 TOA L1C products, an iCOR masking is applied yielding land/water and cloud intermediate layer files. In the next step, AOT values are either retrieved from the S2 image, or obtained from an external dataset, i.e., CAMS data (Morcrette et al., 2009, Inness et al., 2019). The SIMilarity Environment Correction (SIMEC, Sterckx et al., 2015) is applied to correct for adjacency effects which otherwise will make the apparent reflectance of dark targets, such as inland waters, brighter when surrounded by bright pixels, e.g. land. The land/water, cloud, and AOT layers together with MODTRAN5 LUTs, DEM and the solar and viewing angles (mean of the angular values given in S2 metadata file) are used as input for the actual iCOR atmospheric correction. The result is an S2 water-leaving reflectance (RHOW) product.

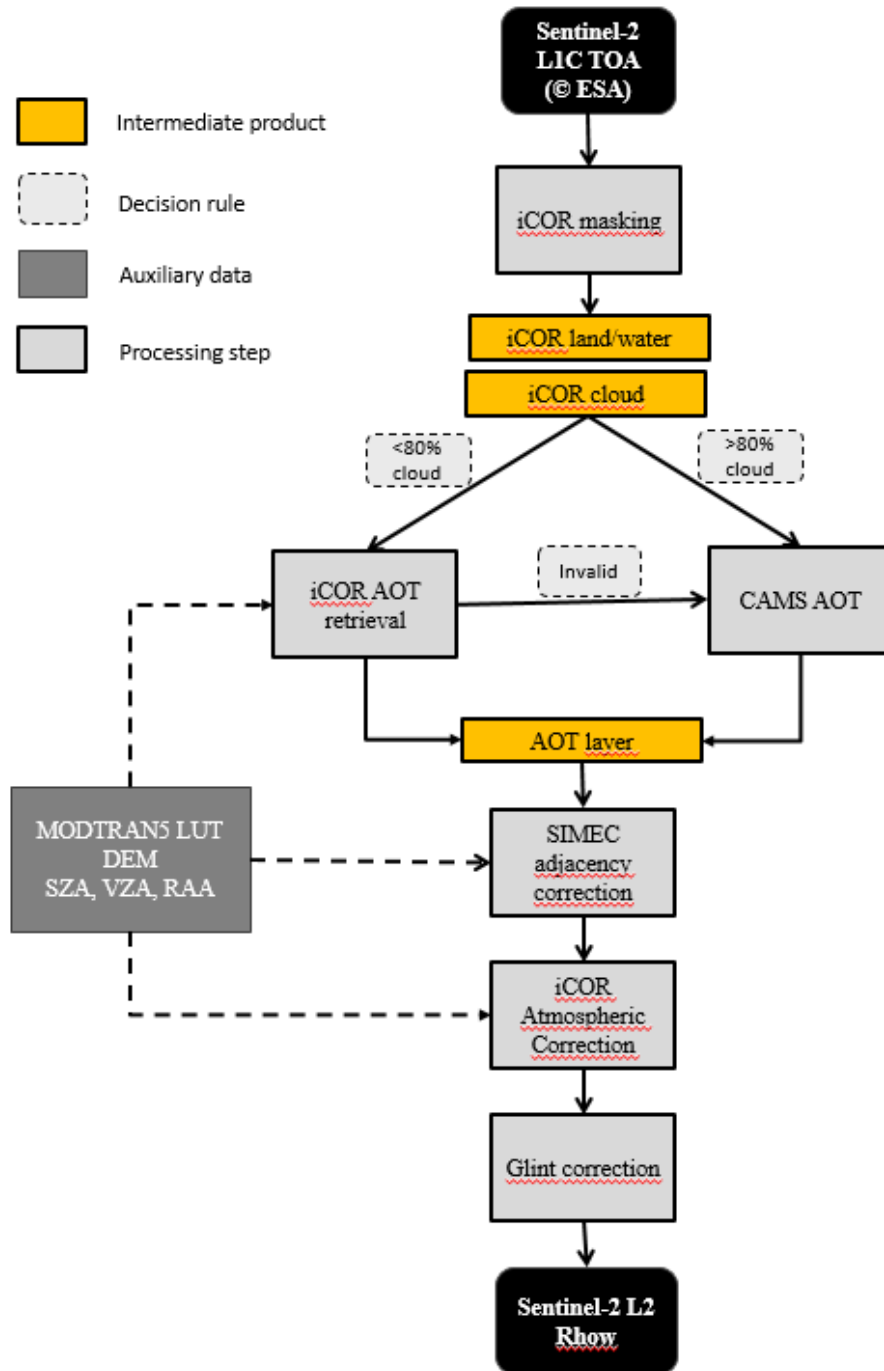


Figure 4.1: Workflow of iCOR implemented in the Terrascope processing chain. The iCOR AOT retrieval is invalid when the absence of clear land pixels hamper an accurate image-based AOT retrieval.

Internal iCOR land/water mask

Discrimination between land and water pixels is required in both the AOT retrieval and in the final atmospheric correction step. Over water an additional sky glint correction is performed. The land-water mask is generated based on a threshold of the TOA reflectance signal in the 10 m NIR band: if the TOA reflectance in Band 8 (842 nm) is lower than 0.05 (-), the pixel is classified as water in the atmospheric processing step. The resolution of this intermediate product is 10 m, which is resampled to 20 and 60 m using nearest neighbour resampling as implemented in the GDAL library.

Internal iCOR cloud detection

An internal cloud detection algorithm is used in the atmospheric correction step instead of the standard Sen2Cor or IdePix cloud mask, because an over-detection of clouds is favoured over a 100 % accurate cloud mask to estimate the AOT accurately. The method for cloud detection is based on the method formulated by Guanter et al. (2008). The method can be applied to all sensors with VNIR bands.

Average cloud reflectance can be assumed to be rather high for all visible bands. In practice, three thresholding values are applied. When these values are exceeded, the pixel is identified as cloud:

- The average TOA reflectance for all VNIR bands (B01 – B08A) is calculated and compared with the ‘average’ threshold value of 0.19 (-).
- The BLUE reflectance (B01 – 490 nm) is compared with the ‘minimum’ threshold of 0.25 (-).
- The reflectance in the cirrus band (B10 – 1375 nm) is compared with a threshold value of 0.01 (-).

The resolution of the intermediate cloud mask is 60 m. In the case of aerosol detection, the cloud mask is dilated with an extra surrounding border of 10 pixels (600 m), to make sure that pixels that are in the vicinity of clouds or that are under-detected are discarded for further use in retrieval algorithms.

AOT at 550 nm

The origin of the AOT data at 550 nm used in the Terrascope atmospheric correction depends on the image quality: by default, the AOT will be retrieved from the imagery using iCOR [RD2]. When the cloud percentage is too high (>80%) or the iCOR-derived AOT is invalid (not enough land or spectral variety), an external AOT dataset will be used. CAMS Near Real Time (NRT) data, as provided by the European Centre for Medium-Range Weather Forecasts (ECWMF) are preferred, unless the time window between S2 and CAMS NRT data becomes too large (> 24 h). Such rare cases can occur as a result of connection issues between the servers. In these cases, CAMS climatological monthly averages (Inness et al., 2019) are used. The fall-back mechanism is depicted in Figure 4.2.

The iCOR image-based AOT retrieval subdivides the TOA image into $\sim 15 \times \sim 15$ km² blocks, large enough to include high spectral variation and small enough to assume spatial atmospheric homogeneity. In a first step, a maximum AOT threshold is set using a dark dense vegetation approach. Next, the AOT value is refined using the spectral variation within the 15 × 15 km² block, using a multiparameter endmember inversion technique. Five pixels with high spectral contrast

(selected based on the NDVI values from TOA reflectance) are represented by a linear combination of three pre-defined default vegetation spectra and a soil spectrum, see Section 2.2.2.

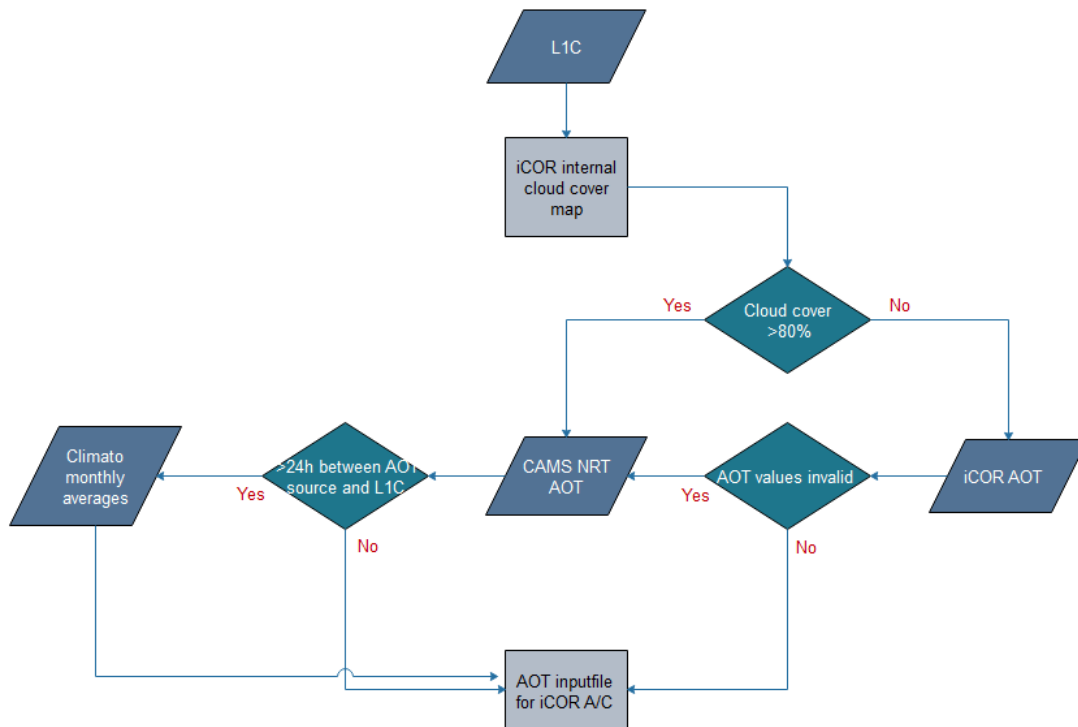


Figure 4.2: Flowchart explaining the AOT origin.

SIMEC adjacency correction

The SIMEC adjacency correction (Sterckx et al., 2015) is based on the NIR similarity (NIR_{sim}) assumption (Ruddick et al., 2006) which states that the shape of the water spectrum in the NIR region is invariant. After normalizing the water leaving reflectance at 780 nm, the value should fall within a predefined range:

$$NIR_{sim} - Stdev \leq \frac{\rho_w^t}{\rho_w^r} \leq NIR_{sim} + Stdev$$

With ρ_w^t and ρ_w^r the retrieved water leaving reflectance for respectively a “test” spectral band and the “reference” spectral band situated near 780 nm. When this requirement is not fulfilled, pixels are assumed to be influenced by adjacency effects. The background radiance for range N is calculated as a weighted average of the pixel radiance values surrounding the target pixel. In an iterative manner, the optimal range (N) for defining the environmental influences is determined, as depicted in Figure 4.3. Sterckx et al. (2011) defined optimal waveband settings for the “test” band as; (i) minimum influence of gaseous absorption, (ii) not lower than 690 nm because of increasing uncertainty, and (iii) preferably located in the red-edge region of the spectrum where contrast between water and land is more pronounced. The availability of spectral bands is a restrictive factor in multispectral sensors. For Sentinel-2, bands 5 (704 nm) and 7 (783 nm) are selected, respectively.

Sterckx et al. (2014) defined restrictions for the use of SIMEC which tends to fail in (i) high turbid waters where the NIR reflectance is flattened (Doron et al., 2011; Goyens et al., 2013), (ii) in waters with macrophyte growth or specific algae blooms, and in (iii) areas where bottom effects are significant in the NIR (optically shallow waters).

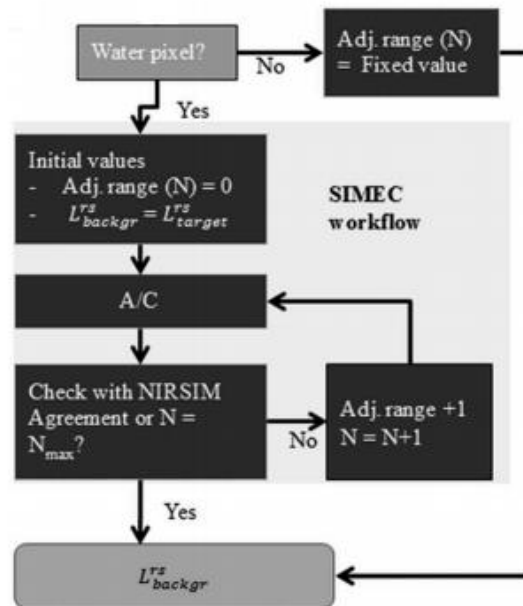


Figure 4.3: SIMEC adjacency correction workflow.

iCOR Atmospheric correction + glint correction

In the next step, all generated input data are inserted into iCOR, which makes use of MODTRAN-5 LUTs (see ANNEX I). The water vapour is fixed at 2.0 g cm⁻² and the aerosol model is fixed at a continental model. Water pixels undergo an additional glint correction, which is a subtraction of the lowest reflectance signal in the RED-SWIR spectral range (B04-B12). Water strongly absorbs in the NIR-SWIR and approaches zero reflectance. The residual signal can be related to some remaining glint effects.

4.2.3. Outlook

iCOR will be continuously updated and improved. Terrascope S2 water will stay up-to-date with the latest iCOR version. If an updated version results in a significant improvement, the Terrascope workflow will be updated accordingly to include the new version and a reprocessing of the archive might take place.

5. Limitations

5.1. Pixel classification

Each new publicly available update of the IdePix scene classification module will be analysed in terms of added value for processing new and historical products compared to previous versions and the required effort for implementation or update. For minor changes, NRT products will be processed with the new version. Only if the cost/benefit analysis is positive to reprocess the full archive, the update will be implemented as well for historical data.

5.2. Atmospheric correction

Each new publicly available iCOR update will be analysed in terms of added value for processing new and historical products compared to previous versions and the required effort for implementation or update. For minor changes, only NRT products will be processed with the updated version. For major changes, a cost/benefit analysis will indicate if a full reprocessing of the historic archive is required.

As iCOR is tile-based, edge artefacts can occur between different tiles acquired on the same date. This is illustrated in Figure 5.1. These artefacts are most pronounced when in one tile the AOT is derived from the image itself, while in the neighbouring tile the AOT CAMS NRT fall back mechanism is activated.



Figure 5.1: Effect of tile-based processing is visible in this example of S2 data acquired on 13/10/2018. The tile edges are highlighted by the white arrows.

6. Quality assessment

6.1. Atmospheric correction

iCOR was part of the Atmospheric Correction Intercomparison Exercise (ACIX-Aqua), a joint NASA-ESA activity, initiated to enable a thorough evaluation of eight state-of-the-art atmospheric correction (AC) processors available for Landsat-8 and Sentinel-2 data processing. The results are publicly available in Pahlevan et al. (2021), only a selection will be presented here to demonstrate the performance of iCOR for inland waters.

Eight different AC processors, applied to Landsat-8 Operational Land Imager (OLI) data and Sentinel-2A/B MultiSpectral Instrument (MSI) images over inland and coastal waters, were evaluated: Atmospheric Correction for OLI 'lite' (ACOLITE), iCOR, Sea-Viewing Wide Field-of-View Sensor (SeaWiFS) Data Analysing System (SeaDAS), POLYnomial-based approach established for the atmospheric correction of MERIS data (POLYMER), Glint Removal for Sentinel-2 (GRS), Case-2 Extreme Waters (C2X), Ocean Color - Simultaneous Marine and Aerosol Retrieval Tool (OC-SMART), and MEETC2. The characteristics and properties of these algorithms can be found in Pahlevan et al. (2021). Figure 6.1 shows the distribution of reference data for validation, which can be categorized into AERONET-OC data, capturing predominantly coastal ocean environments, and the so-called Community Validation Database (CVB), representing primarily inland water observations. This latter dataset was collected through an international community-wide data sharing initiative, with the goal to include optically diverse water bodies in the validation exercise. Since iCOR focuses on inland waters, no validation results with AERONET-OC are included.

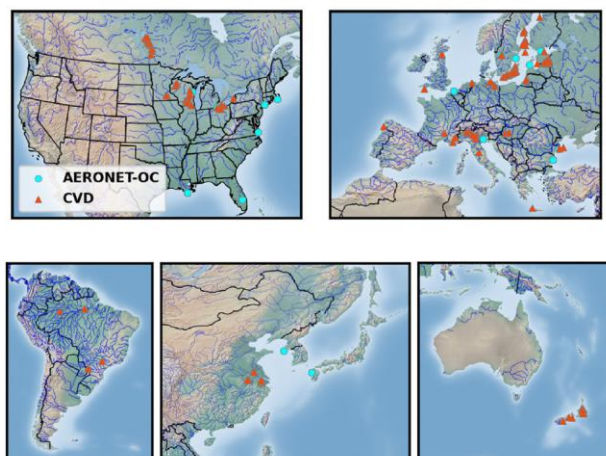


Figure 6.1: Locations of valid in situ radiometric matchups acquired near-coincident with Landsat-8 and Sentinel-2 overpasses. These matchups correspond to diverse aquatic ecosystems, including lakes, rivers and coastal waters. The Community Validation Database (CVD) contains data mostly representing inland waters. Background map source: <https://www.shaderelief.com> (Pahlevan et al., 2021).

Figure 6.2 provides a summary of the median symmetric accuracy (ϵ) and symmetric signed percentage bias (β) for the CVD. The metrics were computed as follows (Pahlevan et al., 2021):

$$\beta = 100 \times \text{sign}(z)(10^{|z|} - 1) [\%] \quad \text{where } Z = \text{Median} \left(\log_{10} \left(\frac{\hat{\rho}_w(\lambda_i)}{\rho_w(\lambda_i)} \right) \right)$$

$$\epsilon = 100 \times (10^Y - 1) [\%] \quad \text{where } Y = \text{Median} \left| \log_{10} \left(\frac{\hat{\rho}_w(\lambda_i)}{\rho_w(\lambda_i)} \right) \right|$$

λ_i refers to spectral band i . The lower the ϵ and β values, the better. The upper plots show the results for the OLI and MSI combined bands. The lower plots show the MSI-specific NIR bands. From these figures it appears that none of the processors appear to uniformly meet the 30 % retrieval accuracy requirements across all bands. The blue bands showed the lowest performance of all VIS bands and nearly all processor underestimate the reflectance in the VIS, with iCOR and ACOLITE returning minimal biases in 490, 560 and 664 nm bands. For the NIR bands, large uncertainties are found for 740 and 783 nm bands and no consistent positive or negative bias are evident across the processors.

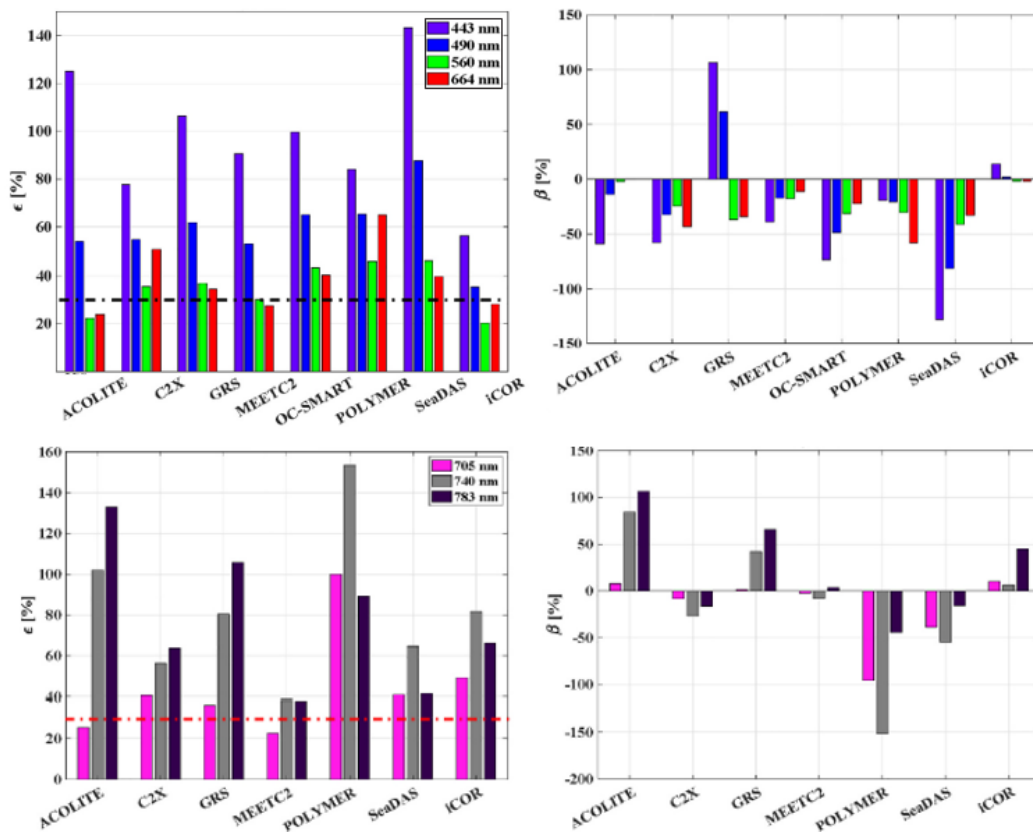


Figure 6.2: Performance assessments as determined by the median symmetric accuracy (ϵ) and median symmetric bias (β) for OLI and MSI matchups combined in the top graphs and only MSI-specific bands in the bottom graph. The dashed lines in the top plot corresponds to a 30% threshold (Pahlevan et al., 2021).

In the next step, the spectra were subdivided into Optical Water Types (OWT), which allowed an assessment of processors across widely variable coastal and inland water conditions. In total seven OWTs were defined: OWTs 1 and 2 are commonly found in the coastal waters and/or oligotrophic lakes. OWT3 is attributed to moderately eutrophic waters. Lakes or coastal estuaries with various degrees of phytoplankton blooms are represented by OWTs 4, 5 and 6. Lastly OWT7 ensures that sediment-rich water are also present. More information about the specification for the water constituents per OWT can be found in Pahlevan et al. (2021).

A pair-wise intercomparison was performed where win rates were calculated per OWT and band for each AC pair. A winning processor for each pair, the one with the lowest ϵ , was assigned with unity. As a result, for each AC pair, a 4 (band) by 7 (OWT)-element binary array filled with 0s or 1s was formed. This pairwise intercomparison was repeated for all the processors to generate seven binary arrays, which were added and normalized by the total number of pairwise comparisons ($N=7$). Having these normalized heatmaps created for all processors, the AC processors are likely to produce the most accurate RHOW for any given band and OWT were determined. The result is shown in Figure 6.2, while Table 6.1 provides the ranking of AC processors specified using band average (column-wise) performances in Figure 6.3.

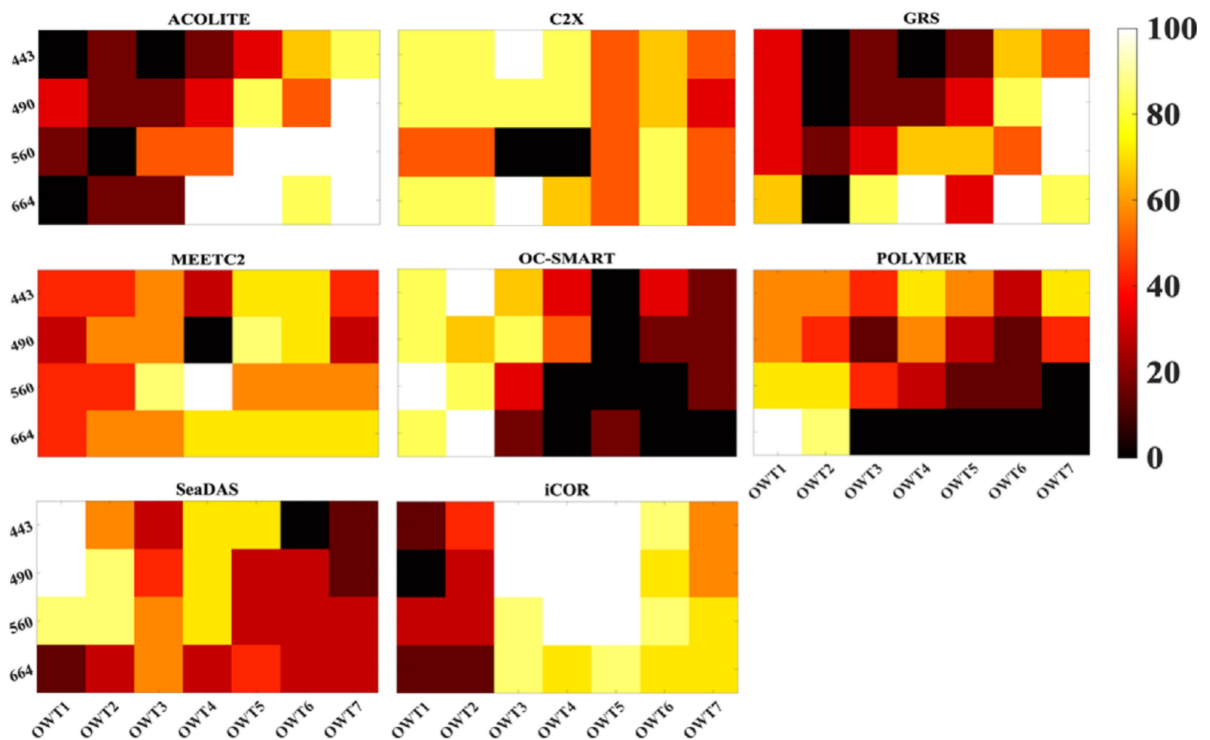


Figure 6.3: Relative performance assessments [%] determined via aggregating pairwise intercomparisons. Processors with bright colours (white or yellow) are likely to generate high-quality $\hat{\rho}_w$ for a given OWT and band (Pahlevan et al., 2021).

Table 6.1: Ranking of AC processors specified using band-average (column-wise) performances in Figure 6.3. Note that iCOR was only analysed using CVD matchups (Pahlevan et al., 2021).

Order	OWT1	OWT2	OWT3	OWT4	OWT5	OWT6	OWT7
1	OC-SMART	OC-SMART	iCOR	iCOR	iCOR	iCOR	ACOLITE
2	SeaDAS	SeaDAS	C2X	SeaDAS	ACOLITE	MEETC2	GRS
3	C2X	POLYMER	MEETC2	C2X	MEETC2	ACOLITE	iCOR
4	POLYMER	C2X	OC-SMART	OC-SMART	SeaDAS	C2X	MEETC2

This global intercomparison exercise shows that there is not one best solution for all inland and coastal water bodies. iCOR and ACOLITE seem to outperform other schemes for the diverse mostly freshwater observations contained within the CVD or in turbid and/or eutrophic ecosystems represented by OWTs 3 through 7. In clearer waters (OWTs 1 and 2), OC-SMART and SeaDas are the best performers.

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ANNEX I – MODTRAN5 LUT input parameters

LUTs of the atmospheric correction parameters and the diffuse transmissions are pre-calculated with MODTRAN 5 in function of viewing zenith angle, solar zenith angle, relative azimuth angle, AOT, column water vapor, elevation, and ozone. The LUT is generated for the standard rural MODTRAN aerosol type, for a sun-to-earth distance in astronomical units of 1.

For the MODTRAN5 runs the DISORT (DIScrete Ordinate Radiance Transfer) option is selected to properly account for the azimuthal dependency of multiple scattering as indicated by Campbell et al. (2011). Berk et al. (2005) showed that the spectral radiance predictions in the visible spectral region (400-700 nm) with ISAACS multiple scattering can be 10% below the results obtained with 8-stream DISORT depending on the atmospheric and observation conditions. The Thuillier *et al.* (2003) [ORD4] sun irradiance spectrum is preferred instead of the standard extraterrestrial solar irradiance models included in MODTRAN. A fixed atmospheric vertical profile (i.e. the default mid-latitude summer atmosphere) is used for the MODTRAN-5 runs.

Two separate LUTs are created, one for Sentinel2-A and one for Sentinel-2B, based on their respective spectral response curves (ESA, 2017).

The breakpoint positions for the different input parameters of the LUT are listed in Table A.0.1.

Table A.0.1: Breakpoints MODTRAN5 LUT.

STEP	1	2	3	4	5	6	7	8	9	10	11
VZA(°)	0	5	10	12							
SZA(°)	0	10	20	30	40	50	60	70	75	80	
RAA(°)	0	25	50	85	120	155	180				
ELEVATION(km)	0.01	1	2	3	4						
AOT@550 nm (-)	0.01	0.05	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	1
CWV (g cm ⁻²)	1	2	3	3.5							
OZONE (atm-cm)	0.33										