TERRASCOPE SENTINEL-2
ALGORITHM THEORETICAL BASE DOCUMENT (ATBD)

S2 – WATER QUALITY – V120

Reference: ***Terrascope Sentinel-2 Algorithm Theoretical Base Document S2 – WATER QUALITY – V120***
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LIST OF ACRONYMS

ACRONYM	EXPLANATION
ATBD	Algorithm Theoretical Base Document
CDOM	Coloured Dissolved Organic Matter
CHL	Chlorophyll-a
DN	Digital Number
FNU	Formazin Nephelometric Unit
iCOR	Image Correction for atmospheric effects
OC	Ocean Colour
OGC	Open Geospatial Consortium
PROBA-V	Project for On-Board Autonomy – Vegetation
RHOW	Water leaving reflectance
S2	Sentinel-2
SAR	Synthetic Aperture Radar
SPM	Suspended Particulate Matter
SPOT-VGT	Satellite Pour l'Observation de la Terre - Végétation
SYN	Synergy
TUR	Turbidity
VM	Virtual Machine
WMS	Web Map Service
WMTS	Web Map Tile Service

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

The water quality parameters Turbidity (TUR), Suspended Particulate Matter (SPM) and Chlorophyll-a (CHL) derived from Sentinel-2 data are offered in Terrascope alongside land and reflectance products.

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 processing steps to go from the Sentinel-2 (S2) Water-Leaving Reflectance (RHOW) data to the water quality products TUR, SPM and CHL, embedded in the Terrascope Sentinel-2 water v120 processing chain.

The document is organised as follows:
- Section 2 provides an overview of all input data needed for the processing workflow.
- Section 3 explains the data available to users.

- Section 4 provides a detailed description of the different algorithms that compose the RHOW to Water Quality workflow.
- Section 5 discusses the implemented algorithm's limitations.
- Section 6 justifies the overall workflow with a quality assessment.

1.3. Description

In the first step of the Terrascope S2 water processing chain, S2 water leaving reflectance (RHOW) products were generates as described in the Terrascope ATBD S2 – RHOW – V120 [RD1].

From the RHOW products the water quality parameters are derived. These are:

- Turbidity (TUR)
- Suspended Particulate Matter (SPM)
- Chlorophyll-a concentration (CHL)

The methodology used to derive the water quality parameters relies on semi-empirical relations from Nechad et al. (2010) , Dogliotti et al. (2015) and an AI algorithm developed by Pahlevan et al. (2020). Details are provided in Section 4.

The document is applicable for the Terrascope S2 water V120 processing chain. Table 1.1 summarizes the main characteristics of the different Terrascope versions until V120. The adaptations between Terrascope V100 and V120 are summarized in Table 1.2.

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

Version	Main characteristics
V100	Input: L1C data WQ algorithms: - CHL: Switching between OC3 (O'Reilly et al., 1998) and Gilerson et al. (2010) - SPM: Semi-empirical relation Nechad et al. (2010), switching as suggested by Dogliotti et al. (2015) - TUR: Semi-empirical relation Nechad et al. (2009), switching as suggested by Dogliotti et al. (2015) Output: CHL, SPM, TUR
V110	Input: L1C data **(adjusted base processing ESA, changes described in [RD2])** WQ algorithms: - CHL: Switching between OC3 (O'Reilly et al., 1998) and Gilerson et al. (2010) - SPM: Semi-empirical relation Nechad et al. (2010), switching as suggested by Dogliotti et al. (2015)

Version	Main characteristics
	- TUR: Semi-empirical relation Nechad et al. (2009), switching as suggested by Dogliotti et al. (2015) Output: CHL, SPM, TUR
V120	Input: L1C data WQ algorithms: - **CHL: Mixture Density Network (MDN) Pahlevan et al. (2020)** - SPM: Semi-empirical relation Nechad et al. (2010), switching as suggested by Dogliotti et al. (2015) - TUR: Semi-empirical relation Nechad et al. (2009), switching as suggested by Dogliotti et al. (2015) Output: CHL, SPM, TUR

Table 1.2: List of changes between TERRACOPE Sentinel-2 V100 and V120

Adaptations between V120 and V100	Clarification
Input data	
Adjusted base processing by ESA.	On 30.09.2021, the ESA base processing was updated. For a list and clarification of changes, see [RD2].
Output data	
Update of approach for CHL retrieval from switching between OC3 (O'Reilly et al., 1998) and Gilerson et al. (2010) to the MDN algorithm developed by Pahlevan et al. (2020).	Based on a validation done using in situ data collected in Flanders and the Netherlands, the better performing MDN algorithm is preferred over the previous switching approach.

1.4. Feature added value/use case

Terrascope provides easy access not only to the basic S2 data, but also the derived products that are generated in a standardized and automated way. In addition, the products are validated. The service allows users to directly derive information on water quality from the S2 data .

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 6.

Table 1.3: List of related documents

[RD1]	De Keukelaere, L., Knaeps, E. (2021). Terrascope Sentinel-2 Algorithm Theoretical Base Document (ATBD) S2 – RHOW – V120.
[RD2]	Gatti, A., Galoppo, A. Castellani, C., Carriero, F. Sentinel-2 Products Specification Document, REF: S2-PDGS-TAS-DI-PSD issue 14.9, 30/09/2021 https://sentinels.copernicus.eu/documents/247904/4756619/S2-PDGS-TAS-DI-PSD-V14.9.pdf/3d3b6c9c-4334-dcc4-3aa7-

1.6. Definitions

The definitions of the water quality parameters are given below.

- **Turbidity** indicates the relative opacity of the water column. It is an optical water property and a measure for the amount of light scattered by constituents the water column. The higher the scattered light intensity, the higher the turbidity. Constituents that causes water to be turbid include clay, silt, very tiny inorganic and organic matter, algae, dissolved coloured organic compounds, plankton, and other microscopic organisms.
  Unit: Formazin Nephelometric Units (FNU) (according to the ISO 7027 method).

- **Suspended Particulate Matter concentration** is the mass concentration of nano-scale to sand size particles which are suspended in the water column. Some particles are present naturally in water, such as plankton, fine plant debris and minerals (sand, silt or clay), while others stem from human activity (organic and inorganic matter). SPM and turbidity are linked: increased SPM concentrations will increase the water turbidity.
  Unit: mg L^{-1} or g m^{-3}.

- **Chlorophyll-a** is a green pigment found in plants. It absorbs sunlight and converts it into sugar during photosynthesis. Chlorophyll-a concentrations are an indicator of phytoplankton abundance and biomass in inland, coastal, and estuarine waters.
  Unit: µg L^{-1} or mg m^{-3}.

2. Input

2.1. Water leaving reflectance

The water quality workflow starts from Water Leaving Reflectance (RHOW). These products are generated in the Terrascope S2 water V120 processing chain [RD1] and are atmospherically corrected using iCOR (De Keukelaere et al., 2018).

The **S2 RHOW Spectral Bands** span the range from the Visible and Near-InfraRed (VNIR) to the Short-Wave InfraRed (SWIR) in different resolutions. The spatial and spectral characteristics are listed in Table 2.1.

Table 2.1: Spatial and spectral characteristics of the S2 RHOW products. Bands used for TUR and SPM in orange shading and for CHL in blue characters.

Layer	Spatial resolution [m]	S2A		S2B	
		Central wavelength [nm]	Bandwidth [nm]	Central wavelength [nm]	Bandwidth [nm]
RHOW-B01_60M	60	442.7	21	442.2	21
RHOW-B02_10M	10	492.4	66	492.1	66
RHOW-B03_10M	10	559.8	36	559.0	36
RHOW-B04_10M	10	664.6	31	664.9	31
RHOW-B05_20M	20	704.5	15	703.8	16
RHOW-B06_20M	20	740.5	15	739.1	15
RHOW-B07_20M	20	782.8	20	779.7	20
RHOW-B08_10M	10	832.8	106	832.9	106
RHOW-B8A_20M	20	864.7	21	864.0	22
RHOW-B11_20M	20	1613.7	91	1610.4	94
RHOW-B12_20M	20	2202.4	175	2185.7	185

The water quality processing chain uses the following RHOW band combinations:

- For TUR and SPM two bands are used (indicated in orange shading in Table 2.1): RHOW-B04_10M and RHOW-B08_20M
- For CHL seven bands are considered (indicated in blue characters in Table 2.1): RHOW-B01_60M, RHOW-B02_10M, RHOW-B03_10M, RHOW-B04_10M, RHOW-B05_20M, RHOW-B06_20M, RHOW-B07_20M.

2.2. WorldCover classification layer

For masking land in the final products, the 2020 WorldCover map is used, see Figure 2.1: (Zanaga et al., 2021). This global land cover map at 10 m resolution provides valuable information for many applications such as biodiversity, food security, carbon assessment, and climate modelling. The map is based on both Sentinel-1 and Sentinel-2 data and is available in Terrascope.

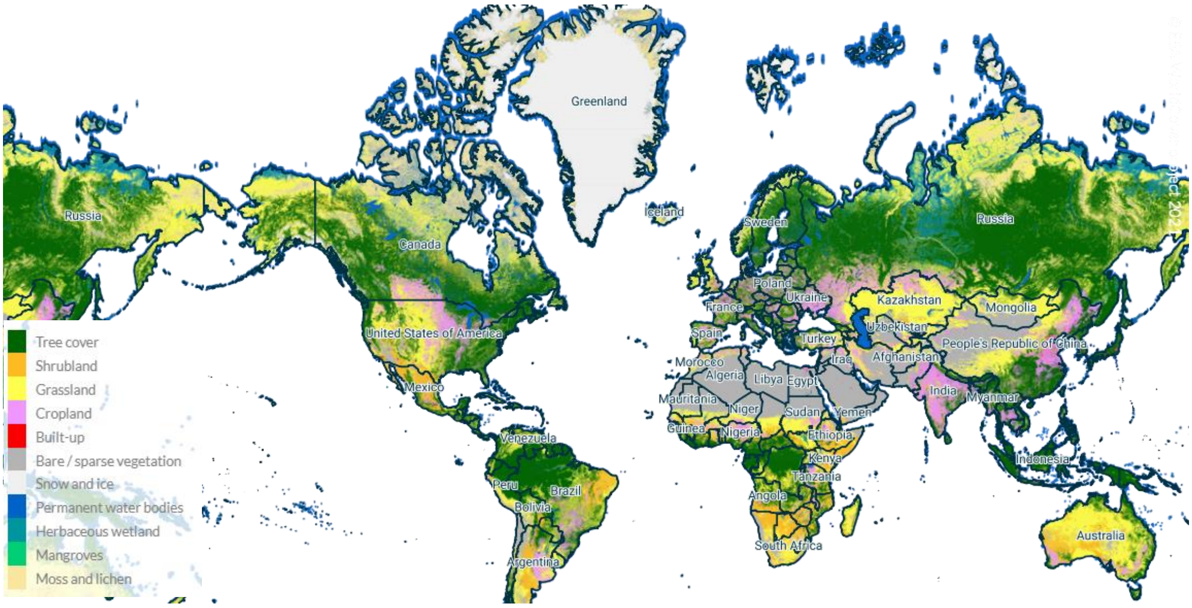

Figure 2.1: Woldcover map (Zanaga et al., 2021).

3. Output

3.1. Product layers

3.1.1. Product data

For the water quality products, the following layers are generated:

- The actual parameter (TUR, SPM, CHL)
- The pixel classification

The files are delivered together with an XML file containing the parameter's metadata. In addition, a quick look file is provided.

TUR and SPM are delivered at 10 m resolution, whereas CHL is only available at 20 m resolution.

3.1.2. Product metadata

The physical pixel values in the S2 water quality files are converted from floating point values into integers, mainly to reduce the file sizes. Table 3.1 provides the technical information of the water quality parameters, like their physical range and the rescaling coefficients. This information is necessary to translate the Digital Numbers (DN) available in the files to Physical Values (PV), using the following formula:

$$PV = DN * scaling + offset$$

Table 3.1: Characteristics of the water quality 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.

	units	Physical min	Physical max	DN min	DN max	offset	slope	No data
TUR	FNU	0	5000	0	50000	0	0.1	65535
SPM	mg L^{-1}	0	5000	0	50000	0	0.1	65535
CHL	µg L^{-1}	0	5000	0	50000	0	0.1	65535

The pixel classification is copied from the RHOW product as described in [RD1]. As mentioned before, the scene classification layer is always outputted in 20 m resolution. Table 3.2 specifies the meaning of the pixel values in this layer. The bands used for masking are indicated are in orange shading.

Table 3.2: Meaning of the values in the Pixel Identification multiband file. Bands used for masking are in orange shading.

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

The folder structure used on the Terrascope platform is:

1. Product and version - *e.g. TUR_V1*
2. Year - *e.g. 2021*
3. Month - *e.g. 09 for September*
4. Day - *e.g. 10*
5. Tile_ID - *e.g. S2B_20210910T105619_31UES_TUR_V120*

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 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:

- Terrascope viewer: https://viewer.terrascope.be/en
  - For viewing, discovery, data access, and data download. The viewer provides fast access to satellite data, including Sentinel satellite data. You can easily search, view, and compare various data layers. Via the ‘Export’ tab you can even download png images, GIF timelapses or the original data in just a few clicks. Would you like to implement your own processing? In that case, you can also directly retrieve the satellite data. You can do so through our data portal.

- 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. TUR and SPM

4.1.1. Justification

Turbidity and SPM are strongly interrelated. Turbidity is an optical property of the water column, and considered as an easily-measurable proxy for suspended particulate matter concentration. SPM and turbidity are an indicator for water clarity, and a macro-descriptor for water quality, since they directly relate to many variables of general use in river and lake water management.

High turbidity and SPM values impact the aquatic ecosystems: they impede light penetration to lower water levels, restricting the rate at which benthic algae, phytoplankton, and macrophytes can assimilate energy through photosynthesis. Shallow lakes and bays can silt and benthic layers smother, affecting living organisms and eggs. Fine particles can clog or damage sensitive gill fish structures and decrease their resistance to diseases. Pollutants, like pesticides and micro bacteria, can cling to the suspended particulates and get transported in the water flow. Water treatment, navigability in channels and longevity of dams and reservoirs are also negatively impacted by high SPM values (Giardino et al., 2017).

4.1.2. Implementation

TUR and SPM are derived using the semi-empirical algorithm of Nechad et al. (2009, 2010):

$$TUR = \frac{A^{\rho}\,\rho_w}{1 - {\rho_w}/{C^{\rho}}}$$

$$SPM = \frac{A^{\rho}\,\rho_w}{1 - {\rho_w}/{C^{\rho}}}$$

with ρ_w the water leaving reflectance for a certain waveband, and A^{ρ} and C^{ρ} are two wavelength dependent calibration coefficients. Both formulas use only a single band in the calculation. However, the sensitivity of each waveband to increasing TUR or SPM is different. For low SPM (< 50 mg L^{-1}), the reflectance at the 665 nm band is preferred as input, while for high SPM (> 150 mg L^{-1}) the sensitivity of this band decreases and saturation can occur. Therefore the reflectance at band 842 nm is favoured for higher SPM. The wavelength dependent calibration coefficients are provided in Table 4.1. A band-switching approach based on work of Dogliotti et al. (2015) is implemented in Terrascope, to tackle both low SPM/TUR and high SPM/TUR waters.

Table 4.1: Wavelength-dependent calibration coefficients to derive TUR and SPM for 665 nm and 832 nm spectral bands.

	A^{ρ}	C^{ρ}
TUR – 665 nm	366.14	0.19563
TUR – 832 nm	1602.93	0.19130
SPM – 665 nm	342.10	0.19563
SPM – 832 nm	1801.52	0.19130

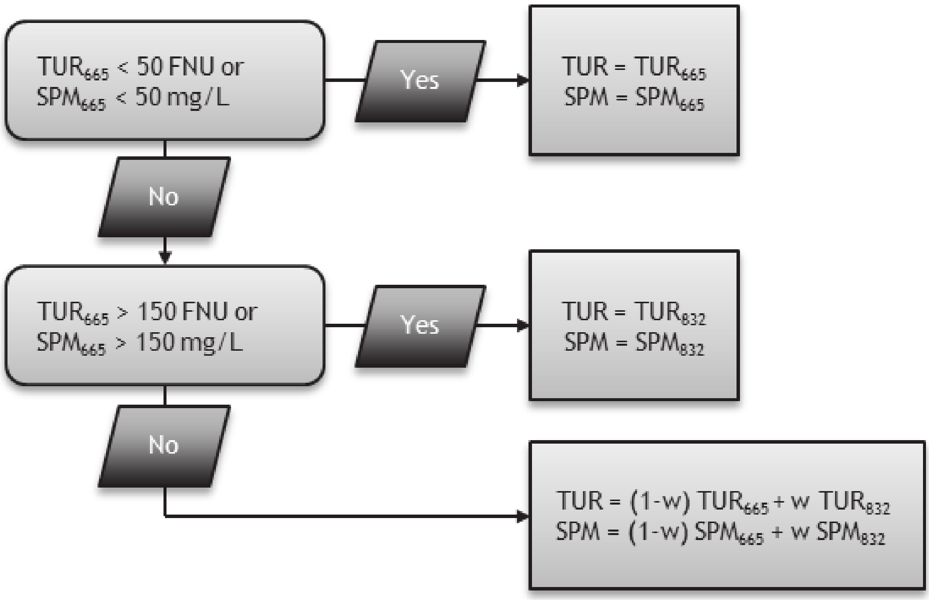

Figure 4.1: Schematic overview of the wavelength switching approach used to derive SPM and TUR. The parameter w is a weighted value: (TUR_{665} -50)/100 or (SPM_{665}-50)/100.

The SPM and TUR products provided in Terrascope are masked using WorldCover (Zanaga et al., 2021) for land masking and IdePix for cloud masking. The IdePix categories selected for masking are marked in orange in Table 3.2.

4.2. CHL

4.2.1. Justification

Chlorophyll-a is a proxy for phytoplankton abundance and biomass in surface waters. Phytoplankton are microscopic, single-celled organisms depending on photosynthesis for energy supply. Both algae (e.g. diatoms and dinoflagellates) and bacteria like cyanobacteria are part of this group. The single cells are hardly observable, but when blooms of thousands or millions of cells arise, they affect the water colour and become observable by human eye or sensor. Phytoplankton form the base of marine and freshwater food webs, produce half of the oxygen that makes our atmosphere suitable for mammals to breathe and are key players in the global carbon cycle.

In coastal and inland waters, chlorophyll-a monitoring is important for management interventions: eutrophication (i.e., increased nutrient loads) can result in dominant algal and cyanobacteria abundance which reduce biodiversity and degrade water quality. The harmful algae blooms can cause health problems in recreational zones or impact potable water (Matthews, 2017).

Chlorophyll-a is included in governmental monitoring programmes:
https://blog.vito.be/remotesensing/an-eye-on-european-waters

4.2.2. Implementation

For the retrieval of CHL, the Mixture Density Network (MDN) suggested by Pahlevan et al. (2020) is used. MDNs fit a mixture of Gaussian distributions, characterized by a mean vector, a covariance matrix and a mixing coefficient vector, to a training data set. The final estimate is obtained by combining the Gaussians, in this case by selecting the estimate corresponding to the highest probability mass.

Pahlevan et al. (2020) trained an MDN on a global dataset of in situ Rrs - CHL pairs and published both the source code and the trained model weights as open source. The model takes reflectances between 400 and 800 nm (B01 – B07) as input, and returns the final CHL estimate.

De CHL products provided in Terrascope are masked using WorldCover (Zanaga et al., 2021) for land masking and IdePix for cloud masking. The IdePix categories masked are marked in orange in Table 3.2.

5. Limitations

5.1. Water quality algorithms

New updates or improved algorithms considered for the derivation of the three water quality parameters 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 algorithms. For major changes, a cost/benefit analysis will indicate if a full reprocessing of the historic archive is required.

5.2. Implementation limitations

Pixels classified in the PIXELCLASSIFICATION layer as ‘Invalid’, ‘cloud-ambiguous’, ‘cloud sure’, ‘cloud buffer’ or ‘cirrus sure’ are masked in the TUR, SPM, and CHL images. Hence, these pixels are set to ‘NoData’ and the TUR, SPM or CHL value is not available. This hampers the use of another user-defined cloud or cloud shadow screening.

WorldCover is used to remove all land from the derived products. Mixed pixels at the borders of rivers and lakes can remain in the end products, but should be carefully considered.

6. Quality assessment

6.1. Terrascope Sentinel-2 CHL product V110 vs. V120

The main difference between the Terrascope Sentinel-2 V110 and V120 versions is the change in the algorithm used for CHL retrieval. This change was made as, based on a dataset of in situ data collected in Belgium and the Netherlands, the previously used algorithm was found to be too unsensitive to changes in CHL.

The in situ dataset used consists of measurements made in both lakes, rivers and the coastal zone in the north of Belgium and the Netherlands. Several datasets were included, i.e. data collected by the Flemish Environment Agency (VMM), the Research Institute for Nature and Forest (INBO), the Flanders Hydraulics Research Hydrological Information Centre (HIC) , the OMES 24-hours and biweekly monitoring campaigns, Rijkswaterstaat (RWS) and Castagna et al. (2022).

From these datasets, Sentinel-2 matchups were selected based on the following conditions:

- Overall cloud cover Sentinel-2 image < 80 %
- For a bounding box of 100x100 m around the measurement location:
  - >= 20% pixels valid OR
  - >= 50% water pixels valid
- Time difference between Sentinel-2 image and in situ measurement < 24 hours

This selection procedure resulted in a set of ca. 2500 matchups. For every matchup, the Sentinel-2 estimate was calculated as the median of the valid water pixels within a 100x100 m bounding box around the measurement location.

Figure 6.1 shows a comparison of the overall validation result of the V110 and V120 algorithms, while Table 6.1 allows to compare both algorithms based on a selection of accuracy metrics. As can be seen in the figure, the V110 algorithm is not sensitive enough to detect changes in the CHL concentration, resulting in severe underestimations. These are caused by a suboptimal algorithm selection in the transition zone between Type I waters, where the OC3 algorithm is applicable, and Type II (i.e. optically complex) waters, where the Gilerson algorithm is applicable. The MDN algorithm (V120) performs considerably better, resulting in a higher correlation, despite an important positive bias. Based on these results, which are in line with values published in literature (e.g. Pahlevan et al., (2020)), the V120 algorithm was preferred over the V110 algorithm.

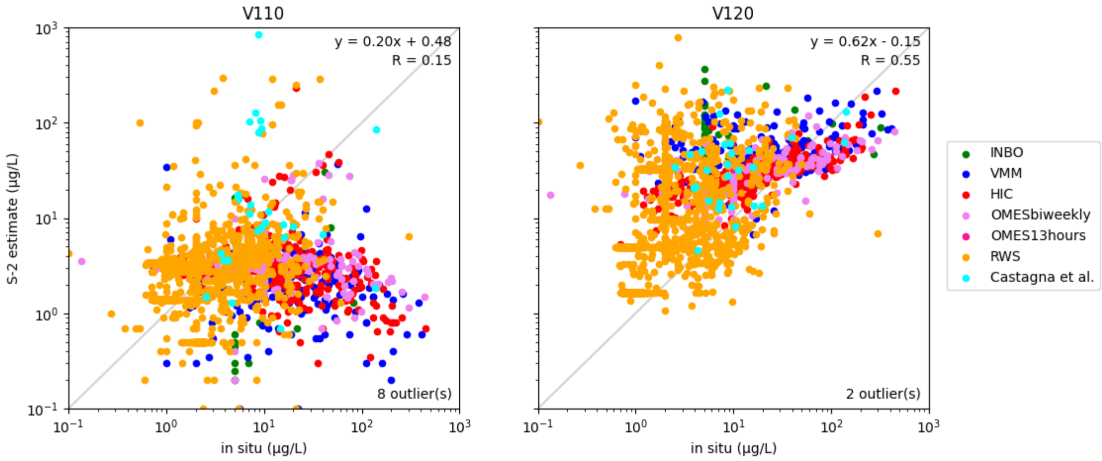

Figure 6.1: Scatter plots of (in situ measurement, Sentinel-2 estimate) for the OC3/Gilerson switching algorithm (V110, left) and the MDN algorithm (V120, right). The plots also display the fitted linear trendline and correlation, both in log scale.

Table 6.1: Accuracy metrics for switching algorithm (V110) and MDN algorithm (V120).

Metric	V110	V120
Correlation	0.01	0.62
Log-Bias	0.650	2.124
RMSLE	0.712	0.687
MAPE (%)	79.0 %	91.7 %

7. Reference documents

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