

Lakes_cci+ - Phase 2 Product validation Plan (PVP)

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1 Introduction and overview

The Product Validation Plan (PVP) defines the approach to the validation of the 6 Essential Climate Variables (ECVs) products of the Lakes ECV developed under the Lakes_CCI project and their associated uncertainties against independent reference measurements, and the intercomparison of the ECV products with other satellite or model data. The PVP is not a public document.

The objectives of the PVP are to:

- define the design of validation activities and the methods used to validate the products and their associated uncertainty estimates.
- describe tools and matchup databases used in the validation process.
- list all reference data sets used to validate each ECV.
- describe the uncertainty characteristics of all reference data.
- describe any limitations in the reference data, such as limited sampling (e.g. clear sky only, daytime only) or mismatches with the satellite measurement conditions, or differences between the reference measurement and the satellite-observed quantity (e.g. skin vs. bulk temperature)
- specify how the validation data were accessed and whether these are open and publicly available or whether these data are protected. If the latter is the case, the data access policy shall be included.
- identify any community validation protocols or standards to be followed.
- define the validation metrics to be used (RMSD, bias, confusion matrices, user/producer accuracies, kappa coefficient., etc.).
- list all satellite and model data sets to be used for intercomparison.
- discuss any mismatches between the ECV products and the data sets used for intercomparison (e.g. different observing times, different resolutions, etc.).



2 Lake Water level – LWL

2.1 LWL validation activities

Two types of validation are performed for LWL.

- 1. Comparison of LWL products against available in-situ observations.
- 2. Dedicated field work in the framework of satellite altimetry calibration / validation programmes.

The comparison with in-situ measurements is done in collaboration with the SHI (State Hydrological Institute in St Petersburg) which is an external partner to the Lakes_cci and which further collaborates in the framework of the Hydrolare lake database.

2.2 Schedule for LWL validation

Validation activity	Time frame for analysis	Implementation
Method 1: direct comparison between LWL products against in- situ data	For most of the lakes the first data were acquired in the 1990s and the last are obtained in recent years (2015 to 2022). Some in-situ data are constantly acquired (in North America in particular) and regular updates of the database are planned.	For method 1 and 2 the methodology is already implemented, and results are updated yearly for both approaches.
Method 2: field work planned at specific dates with corresponding satellites coverage over Lake Issykkul, where all correction steps in LWL processing are checked against acquired in-situ measurements (wet and dry troposphere, instrumental biases).	Yearly field work over Lake Issykkul has been performed since 2003.	

Table 2-1 Overview of LWL validation activities

2.3 Inputs and methods for LWL validation

Multiple in-situ datasets representing various targets around the world are used. These external sources are indicated in Table 2-2. RMS of differences, absolute bias, and potential drifts are produced lake by lake.

Table 2-2. in-situ d	latasets used in	assessment of th	e LWL product.

Source	Description
U.S. Army Corps of Engineer ³	The U.S. Army Corps of Engineer provides in-situ data on Great Lakes. All levels are referenced to the International Great Lakes Datum of 1985 (IGLD 85). Water levels have been coordinated with Canada for 1918-2018.
Hidricos Argentina₄	The database base of Hidricos Argentina provides in-situ data on national rivers and lakes.
U.S. Geological Survey⁵	The USGS investigates the occurrence, quantity, quality, distribution, and movement of surface and underground waters, and disseminates the data to the public. It provides in-situ data on U.S. lakes.



Source	Description
Water Office of Canada	The Water Office of Canada provides historical water level collected over thousands of hydrometric stations across Canada.
<u>FOEN</u> ⁷	The Swiss Federal Office for the Environment provides hydrological data, and in particular the water levels of lakes in Switzerland.
<u>ANA</u> ⁸	The Brasilian "Agencia Nacional de Aguas e Saneamiento Basico" (ANA) provides in-situ data on reservoirs in Brazil.

First, interpolation of the LWL product to the dates of in-situ measurements are performed. Subsequently, the mean bias between in-situ and satellite time-series is calculated. Bias is always present since satellite time series and in-situ measurements do not use the same geodetic reference frame. Some results of these comparison are given in Cretaux et al. (2016) and Ričko et al. (2012).

Drift can subsequently be adjusted if it is observed. Root-mean-square differences are calculated, and in case of multi-satellite data the RMS will be derived for each individual mission.

We can see the result for Lake Huron in Figure 1 below.





The second approach is based on 18 years of field work experiments over Lake Issykkul in Central Asia. This large lake (6000 km²) was selected in 2004 to serve as a dedicated calibration / validation site for satellite altimetry over lakes. It has the advantage of overpasses by all past, present and future altimetry missions. The instrumental concept for the field work is widely described in several publications (Cretaux et al. 2009, 2011, 2013, 2018, Bonnefond et al. 2018). In brief, the field work is organised yearly or bi-yearly after consulting the ephemerides of the satellites. GPS levelling of the lake surface is performed along the satellite tracks using a GPS system. In-situ fixed instrumentation allows to assess the stability of the LWL product, and also to validate the atmospheric and geodetic corrections. The main purpose is to perform full error budget analysis including the range measurements using different retracking algorithms (so called ice-1, Ice-2, ocean) and the different corrections (ionosphere, troposphere, geoid).



Figure 2 shows an example of LWL altimetry measurements against LWL from GPS levelling along two tracks (666 and 707) of sentinel-3A.



Figure 2 LWL altimetry measurements compared with GPS levelling along two S3 tracks.

2.4 Known constraints for LWL validation

The main difficulty for LWL validation using the first method is that in-situ measurements are difficult to obtain, so there are few datasets. Validation against one lake may not be relevant for other lakes since we can observe large differences depending on the morphology of the lake, the geographical and climatic conditions. So, using the existing list of in-situ data is not representative of the general accuracy of satellite altimetry for LWL measurement.

Moreover, the inter-comparison between the two types of datasets is also complicated because the insitu measurements have generally discreteness to monthly average values, while the frequency of the satellite flight over the lake is fully determined by its orbit. This requires interpolation, which can also be a source of error, especially when the lake water level variations are sudden or dramatic, or in presence of seiche for example. Although they are considered the ground reference, in-situ measurements are also subject to (generally unknown) measurement uncertainty (data gaps, human error in collecting the data).

Regarding the second approach, in-situ data are collected manually so the comparisons are valid only for a few dates (once or twice per year) and for the specific site visited. The objective is not general validation of LWL but error budget in a well-known case study. The methodology of calibration / validation based on in-situ GPS levelling is moreover quite complex to perform and can be expensive. It is currently funded by CNES as part of the satellite altimeter calibration/validation programme (CALVAL) for the Issyk-Kul site. Additional plans to perform the same experiment over lake Baikal were abandoned due to ongoing difficulties to travel there.

The uncertainty given within the products are not directly relying on the validation process described above. Indeed, validation only allows providing general overview of errors budget (for in site Calibration /



Validation experiment) and comparisons against in-situ data give another overview, but of accuracy in an as relevant as possible context (size, morphology of lakes, environmental conditions). Uncertainties given in the products for LWL are simply the quantification of the dispersion of the individual measurements along the track of the satellites after all corrections have been performed and the average LWL has been calculated. The values of uncertainties are the therefore simply the RMS of the differences of these individual measurements against the average LWL calculated. Results of validation process described here are published and allow users to rely on a degree of confidence of the product, but this cannot be considered as direct uncertainty since the validation is evidently limited to a small number of lakes.

Moreover, uncertainties being only statistical, eventual biases or long-term drifts are not directly visible in these numbers. That is the reason why regular external validations are done. Instrumental biases are extracted from the field experiments, while drifts or seasonal errors due to changing climate (presence of ice for example, or of aquatic vegetation) can be seen with comparison to in-situ historical data.



3 Lake water extent -LWE

3.1 LWE validation activities

The aim of the LWE validation activities is to lend confidence to lake area products and lakes vectors extracted from Sentinel-2 and Landsat images using the ExtractEO processing chain.

Three methods are identified to validate the Lake Water Extent products:

- 1. Cross-validation of coincident very high resolution (VHR) and high-resolution (HR) optical measurements of water extent
- 2. Validation via the hypsometric method against in-situ lake water level measurements
- 3. Validation via the hypsometric method against altimeter estimates of lake water level

The first approach gives a pixel-wise comparison of the VHR and HR products. The two sources must be cloud free and coincident within a short time window. The images should cover, where and when possible, the targeted lake as a whole, including immediate surrounding areas. In the case of large lakes, only part of the lake is covered by both sensors, which presents a specific challenge. Furthermore, VHR are relatively costly, and their use is subject to scrutiny. These validations are, therefore, done over a limited set of lakes representing different environments (Sahelian, temperate tropical, etc) and including fully filled, floodplains, reservoirs, and shallow waters. The result of validation, in this context, is a pixel-wise accuracy estimate, as well as overall aggregated accuracy estimates.

The other two methods are closely related, whilst the use of in-situ measurements is expected to provide more accurate reference than satellite altimeters. On the other hand, in-situ measurements are relatively scarce and therefore limit the scope of this validation approach. The methods give an overall error estimate of the area per classified image, provided that the hypsometric curve can be estimated with high accuracy. We can also estimate the overall area uncertainty.

3.2 Schedule for LWE validation

Validation activity	Time frame for analysis	Implementation
Direct comparison between VHR and HR optical imagery over selected lakes	2022-2023	CDR v2.1 & v3.0
Comparison against in-situ data for lakes where in-situ LWL measurements area available	2023-2024	CDR v3.0
Comparison against altimeter measurements of LWL over all lakes	Variable depending on range of level variability.	CDR v3.0

Table 3-1. LWE Validation schedule.

3.3 Inputs and methods for LWE validation

Cross validation of VHR and HR imagery

An example of cross-comparison between Sentinel-2 (S2) and Pleiades NEO (SPL NEO) is shown in Figure 3. By combining many such pairs of HR and VHR observations we can estimate the accuracy of generating water extent from HR optical imagery. This approach is carried out over different environments: temperate lakes surrounded by cultural parcels and forest, lakes in the Sahelian belt, in the temperate US, with surrounding agricultural parcels, and in China.



The case of Shenjing Lake in Anhui province in China, illustrates the difficulties to extract water extent in shallow waters, when the delimitation of water and wet sediments can be very delicate.



Figure 3 Comparison between Sentinel2 and a Pleaides NEO water extent limit, respectively in yellow and red; the overall accuracy is 98,82%.



Figure 4 Comparison between Pleaides NEO water extent limit (black line) and Sentinel2 for two parametrizations (yellow and orange), with a respective precision of 0.85 and 0.67.



Method 2: Validation via the hypsometric method against in-situ lake water level measurements

In this method we use time-series of S2 LWE estimates and align them with accurate in-situ LWL measurements. This allows us to calculate the regression between LWL and LWE (hypsometry) including the resulting model accuracy.



Figure 5 Hypsometric curves computed for Lac de Der (France) with LWE derived from Sentinel-2 time series and LWE from in-situ data (orange dots) and altimetric data, i.e. Json 3 (blue dots).

Method 3: Validation via the hypsometric method against altimeter estimates of LWL

In the third method, we use the hypsometry analytical function (linearly or polynomial fit) to calculate the LWE variable once a measurement of LWL has been performed and produced. To invert the polynomial coefficient, we need to use a set of vectors at different dates (LWL, LWE) measured using the satellite altimetry for LWL and the satellite imagery for LWE. We generally limit the number of vectors (LWL, LWE) to 10 to 15 per lake, which in general is sufficient to cover the range of variability in water level and extent. Another way of validating the method is to calculate the RMS of the differences between the measured values of LWE (from satellite imagery processing) minus the theoretical value of LWE (calculated using hypsometry function).

This is done for all lakes. In Figure 6 an example for Argyle Lake (Australia) is given. The RMS is expressed in km² which in this case represents less than 1% of the total surface of the lake. Another example shown in Figure 7 shows the results obtained over Nganze lake in China.





Figure 6 LWE vs LWL in Argyle Lake in Australia with a RMSE of 8.13 km², or uncertainty of 0.73%.



Figure 7 LWE-LWL regression for Nganze (PR China) based on the exploitation of two Sentinel-2 tiles. A polynomial fit of the third order gives an overall RMSE=2.39 km² or uncertainty of 0.48%.

3.4 Known constraints for LWE validation

Only method 3 will deliver validation results for all selected lakes. Method 1 hinges on the creation of new datasets. An obvious drawback with method 1 is that we compare two EO datasets, where it can be subjective to determine which is most correct, particularly in case of shallow water surrounded by wet muddy banks. There is a need for a thorough visual inspection of the two products as well as derived metrics. In practice, it is very challenging and costly to gain access to such data over lakes where we have simultaneous acquisitions of VHR and HR cloudiness images.

The main drawback for method 2 is that in-situ measurements of LWL are difficult to obtain, so there are few datasets. Validation against one lake may not be relevant for other lakes since we can observe large differences between the algorithms for different lakes/different conditions.

The main drawback using altimeters is that the accuracy of altimeter data is variable, and expectedly poorer than in-situ data. Also, the fact that altimeters are not synchronized in time with Sentinel-1 and Sentinel-2, adds to the uncertainty.



4 Lake surface water temperature – LSWT

4.1 LWST validation activities

LSWT validation consists of comparing retrieved water-surface (skin) temperature with in-situ temperature measurements, which are obtained at a point within the surface area to which the retrieved temperature applies. This means that LSWT is validated at full satellite resolution (L2 internal products, per pixel) and at L3 (on the gridded 1/120 degree LSWT product).

In-situ temperature measurements in lakes are not common, and the key activity for this purpose is obtaining the maximum number of in-situ data points for comparison. There is no international system for data sharing of in-situ LSWT measurements, and over many years (within the projects ARC Lake, GloboLakes, EUSTACE, CGLOPS and C3S) the team has developed a network of professional connections who share data for our validation use. The collection happens once a year, towards the end of the calendar year. Only data that have at least daily temporal resolution are considered. A significant effort is required to re-format the data received into a common format. Data were obtained in the last effort for 155 observation locations covering 81 lakes that can be remotely sensed (see Figure 8), but this should slowly increase year by year.



Figure 8 Locations of 155 in 81 lakes that can be remotely sensed for LSWT using 1 km infrared imagers such as SLSTR.

The validation of the L2 product will also give de facto the validation performance for the merged product, since these are at effectively the same spatial resolution.



4.2 Schedule for LWST validation

Validation activity	Time frame for analysis	Implementation
Collection of in-situ data from professional network	November/December every year	All inputs reformatted to a standard specification and quality controlled
Matching between in-situ data and L2 and L3 LSWT products	3 months after product generation	Matches are added to a match-up database
L2 comparisons and L3 comparisons	5 months after product generation	Global and per-lake statistics and plots stratified by quality level are generated
Documentation	PVR deadlines	Present results in Product Validation Report

Table 2 LSWT validation schedule.

4.3 Inputs and methods for LWST validation

The collected in-situ data contain as a minimum daily resolution LSWT (preferably sub-daily) with time, longitude and latitude. Metadata on depth is preferable, but data are accepted if we are confident they are surface data even if depth metadata are absent. We have no control on the variety of in-situ instrumentation, but essentially all are thermistor measurements. We do not generally have specific uncertainty estimates for the in-situ measurements or their location, but typically thermistors have uncertainty <0.25 K and locations are specified to well within the 1 km pixel of the highest resolution satellite observations.

In-situ data are quality controlled by ensuring they do not stray too far from a climatology (based on the v3 LSWT product) or fluctuate unphysically quickly (see Figure 9).



Figure 9 Illustration of quality control results, in this case for Lake Huron in year 2002. The red line is the received in-situ data: when thin, this indicates periods failing quality control, and when thick, data that pass quality control. The black line and grey band show the climatological annual cycle for this location and its inter-annual variability (one sigma).

Quality controlled in-situ data are matched to L2 and L3 data (i.e., valid, clear-sky LSWTs), using the criterion that the in-situ data fall within the area of the satellite observation and within 1 day time separation (or are daily mean data). The products are validated by quality level and by minimum quality level, using two standard tables (Table 3 and Table 4) shown below (with purely illustrative numbers).



Table	3:	Validation	statistics	bν	quality	level	
labic	٠.	<i>vanaucion</i>	Statistics	~,	quanty		

	Median	RSD	Mean	SD	Ν
ql=5	-0.300	0.430	-0.389	0.935	2749
ql=4	-0.440	0.652	-0.590	1.242	1827
ql=3	-0.745	1.082	-0.946	1.620	900
ql=2	-1.445	1.749	-1.636	1.945	308
ql=1	-3.310	4.018	-4.110	4.342	1552

Table 4: Validation by minimum quality level

	Median	RSD	Mean	SD	Ν
ql>3	-0.340	0.504	-0.469	1.073	4576
ql>2	-0.370	0.578	-0.548	1.193	5476
ql>1	-0.390	0.608	-0.606	1.268	5784
ql>0	-0.510	0.860	-1.347	2.703	7336

These two forms relate to how users may use quality level information. For example, a user may wish (as we recommend) to use all data with quality level 4 and 5.

The statistics are: median difference; robust standard deviation of difference, calculated as 1.27 times the median absolute deviation from the median; mean; and standard deviation. The median and RSD are less influenced by outliers.

Note that the expected median difference is in the range -0.15 to -0.25 K, because of the water skin effect whereby the thin (~0.1 mm) surface layer of the water body is cooler than water below because (typically) of heat loss from the lake to air but it can vary from lake to lake [Hondzo et al, 2022], [Wilson et al, 2013].

The methods for L3 validation are essentially the same, with the gridded data substituted.

Optimal estimation is used for LSWT retrieval, and this method returns an estimated retrieval uncertainty according to standard equations. These results are then used to provide internal uncertainty estimates for the gridded products. The uncertainty estimates assume Gaussian statistics and in principle could be validated against the robust validation statistics (RSD in the tables).

The RSD of satellite-in-situ difference is explained by three terms (to be added in quadrature): the retrieval uncertainty, the in-situ uncertainty and the consequences of true geophysical variability between the satellite and the match (match uncertainty). Quantitative validation of the retrieval uncertainty from the RSD difference requires additionally precise knowledge of the other two terms. For the case of LSWT validation data, neither of these terms is well quantified, because the validation data are collected from an informal network of contacts and are collected using an unknown variety of sensors and sample-location methodologies. A lower limit on the combined in-situ measurement and match uncertainties comes from analogy with sea surface temperature matches to drifting buoy matches in the open ocean, which have been intensively studied: the lower limit is 0.2 K accounts for in-situ and match uncertainties combined. This in turn places an upper limit on the retrieval uncertainty of LSWT of 0.38 K (for ql = 5). The provided internal uncertainties vary around 0.35 K, so this, as far as it goes, is consistent.



4.4 Known constraints for LWST validation

The principal constraint is the number of remotely-sensible lakes with in-situ data, which is limited. So, for example, the total number of matches for the whole AATSR mission (10 years) for all lakes is around 7300. Also, in-situ data are measured with different instruments, the uncertainty is not known most of the time and sites have different frequency from 15 minutes to twice a year and the time of measurement and/or exact location of the measurement is not always (properly) recorded.

4.5 LWST references

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5 Lake water-leaving reflectance - LWLR

5.1 LWLR validation activities

Validation of LWLR concentrates on the atmospherically corrected LWLR and derived opticalbiogeochemical water column properties, including chlorophyll-*a* and turbidity.

The processing chain for the variables derived from LWLR includes a dynamic mapping of algorithms depending on lake Optical Water Type (OWT). The benefit of this approach over choosing a single algorithm or regional adjustments is that in-situ data belonging to the same optical water type can be pooled together from geographically different sources to firstly calibrate and then validate the system for that OWT. This also means that the algorithm is then expected to perform equally well over waterbodies exhibiting the same OWT, but for which no in-situ data are available, which constitute the vast majority of waterbodies.

Validation activities in Lakes_cci take the form of round-robin comparisons where algorithm selection is not yet established as a result of prior research, typically followed by algorithm optimisation resulting in per-sensor and per-OWT algorithm definitions and associated uncertainty models.

Ultimately, the procedure followed per sensor, per variable of interest and per OWT depends on the availability of in-situ matchup data, which is typically scarce. The following considerations are important when selecting data for validation of LWLR:

- The variable of interest, either LWLR from in-situ radiometry or a biogeochemical or physicochemical component of the water column
- The sampling depth, and whether it can be assumed to represent the water column that is visible from the remote sensor
- The (expected) accuracy of the in-situ measurement
- The sampling location, particularly whether close to shore or on open water
- The time window allowed for in-situ and satellite comparison, which depends on whether absolute (narrow window) or relative performance between algorithms (wide window) is evaluated. Typically, the time window will vary from ±1 to ±7 days, with shorter windows preferred where sufficient reference data can be found.

5.2 Schedule for LWLR validation

Due to scarcity of in-situ data, specific algorithm calibration, validation and uncertainty characterisation was previously not carried out for the OLCI observation period, which is instead based on propagation of MERIS algorithms and performance. In recent years, with the increasingly operation period of OLCI and the emerging of new algorithms, a full validation of OLCI algorithms is scheduled, with results planned to be used in CRDP v3.0.

For the MERIS and MODIS sensors, LIMNADES and GLORIA datasets now contain sufficient observation data for algorithm calibration and uncertainty characterisation, based on initial estimates. Further investigation of the optical variability in these data sets is required to establish whether end-to-end validation is possible for each optical water type used to select algorithms during processing, and whether this can be done in addition to algorithm calibration. Table 5-1 lists the priorities in terms of calibration, validation and uncertainty characterisation with their intended time frame, from the start of the Lakes_cci to present plans. The current priority is to perform algorithm calibration exercise and uncertainty characterisation for OLCI.



Table 5-1 LWLR Validation schedule.

Validation activity	Time frame for analysis	Implementation
Algorithm calibration and uncertainty characterisation for MERIS	Completed in project phase 1 (2018-2022)	MERIS and OLCI (propagated) algorithms and pixel uncertainties in CRDP v1.0
In-situ matchups with MODIS and MERIS observations. A round-robin evaluation and selection of atmospheric correction methods.	Completed in project phase 1 (2018-2022)	MODIS evolution of the processing chain for CRDP v2.0
Algorithm calibration and uncertainty characterisation for MODIS	Completed in project phase 1 (2018-2022)	MODIS algorithms and pixel uncertainties in CRDP v2.0
Cross validation between LIC, LWST and LWLR (conducted as part of consistency option)	Analysis completed in project phase 1, (2018-2022), implementation with CRDP v2.1	Including a climatologic filtering module and a LWLR quality band in CRDP 2.1
Algorithm calibration exercise and uncertainty characterisation for OLCI	Jun 2023 – July 2025	OLCI algorithms and uncertainties CRDP v3.0
Atmospheric correction upgrades across all sensors	Nov 2022 - Oct 2024	Upgrades will trigger re-evaluation of algorithm tuning and uncertainties, per sensor.

5.3 Inputs and methods for LWLR validation

We recognise two separate sources of in-situ validation data: those collected as part of national monitoring programmes and those collected by research institutes for biogeochemical or bio-optical research. Challenges with statutory monitoring data include shore-based sampling which has very limited value as reference for optical remote sensing, and common lack of accuracy in recording sampling locations (often documented as static but in practise varying). Furthermore, such data sets are invariably limited to biogeochemical and physicochemical observations, therefore only supporting end-to-end validation of biogeochemical products without validating LWLR along the way. This is a problem because the dominant source of uncertainty in the final product is assumed to be the atmospheric correction which can only be established by having reference measurements of LWLR. Language may form a further accessibility barrier in accessing these data sets, and therefore geographic bias is a further issue. For these reasons, very few data sets from national monitoring programmes have been successfully incorporated in large scale satellite matchup activities. National monitoring data sets are being increasingly made open access, so their uptake may increase in future.

The challenge with existing research-quality in-situ data sets is that these originate from a scattered landscape of limnological research laboratories using varying measurement protocols (not always documented) and a widely varying set of license terms and accessibility issues. The effort associated with ensuring licenses are established and then honoured when resulting in reports and publications is substantial. To overcome some of these obstacles, LIMNADES, a community-owned bio-optical data archive hosted by University of Stirling, was launched during the UK-GloboLakes project, with many research teams contributing in-situ campaign data. License terms were updated in 2019 to support wider use of the data set. Because the LIMNADES initiative was not initially a funded activity and the effort of collating and harmonising the contributions is substantial, private and public access to the data has remained poor. LIMNADES primarily includes observations from inland water bodies and additionally includes some near-coastal observations.



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A recent re-assessment of community contributions resulted in the GLORIA dataset (Lehmann et al. 2023), a quality-checked static dataset of lake observations specifically including LWLR and one or more supporting bio-geo-optical reference analyses.

It should be clear from the above that the community-owned datasets are the result of global efforts which include subtle methodological differences. The uncertainties associated with this variability in methodology is *a priori* unknown. In GLORIA, reproducibility of results is addressed for part of the dataset (providing average and coefficient of variation) whereas, for another part of the dataset, reconstructed LWLR from in-situ (ir)radiance measurements compared to the reported LWLR resulted in bias estimates at LWLR peak amplitude in the order of +6%.

Validation and uncertainty estimation are closely linked for LWLR, as described in the next section. In brief, validation results are based on matchup analysis resulting in statistical metrics of correlation, whereas the uncertainty propagation models express the statistical performance as a function of the similarity of the satellite-derived LWLR spectrum to OWTs.

5.4 Known constraints for LWLR validation

Because some OWTs are more commonly observed than others and because in-situ bio-optical and remote sensing research in the last decades strongly focussed on waterbodies suffering the effects of eutrophication, it is not possible to produce a set of satellite matchups for each OWT that is sufficiently large to separate calibration, validation and uncertainty characterisation. This situation is gradually improving with the inclusion of new and recovered datasets.

Validation and product uncertainties

The E3UB v2.1.1 document describes in detail why and how product validation and product uncertainty are necessarily linked for LSWT and derived variables. In brief, the application of fuzzy pixel classification and algorithm selection in combination with non-linear optimization techniques favours statistical uncertainty characterization on the final product over analytical error propagation. In addition, in-situ reference data to inform uncertainty characterization are unlikely to cover the range observed in nature. The use of in-situ data for uncertainty characterization has two implications for the validation of the products and product uncertainty itself:

- The uncertainty characterization approach must take the range of the in-situ reference data into account, i.e. extrapolation of product uncertainty beyond the value range of the validation data shall not be allowed. Ultimately, uncertainty maps will thus also in a spatial sense reflect regions where product uncertainty is not yet known. This can then guide further field work (into affected and/or new optical water types) contributing to both product validation and broader uncertainty reporting.
- Uncertainty in the in-situ validation data, due to the use of different (even if optimised) protocols by contributing research groups, will contribute to product uncertainty. Divergence in observation protocols is likely to show as systematic bias that is different between contributed datasets – at present this is expected to be a minor effect. Another effect stems from divergence in instrument deployment protocols, such as the frequency of maintenance or the distance from shore at which samples are taken, which could introduce more significant bias.

OLCI Algorithms validation and calibration

Normally, water quality algorithms are calibrated and fine-tuned using in-situ concentration measurements and hyperspectral radiometric data collected on-site. However, it is crucial to acknowledge the significant challenge posed by atmospheric correction when estimating water quality parameters remotely. A study focused on Chla suggests that atmospheric correction can lead to a performance loss of at least 30% (Pahlevan et al. 2021). This performance loss could be larger on



Turbidity (based on single waveband retrieval), considering that band-ratios used in Chla algorithms may better cancel out the potential systematically bias after atmospheric-correction. Consequently, when these algorithms are directly applied to satellite data, their performance may be compromised.

To tackle this challenge, further calibrations using reflectance data derived from satellites are implemented for the algorithms currently used in Lakes_cci. This additional tuning step aims to mitigate the systematic biases introduced by the atmospheric correction process. By incorporating satellite-derived reflectance data, the algorithms can more effectively account for and mitigate the influence of atmospheric effects. This, in turn, enhances their performance in accurately estimating water quality parameters.

However, it is worth noting that some machine-learning-based algorithms which will be included in the upcoming OLCI algorithms validation may not be suitable for, or not require, additional tuning. Despite the limitations in further tuning for these algorithms, efforts should still be made to address the atmospheric correction challenges and improve their overall performance in water quality estimation.

5.5 LWLR references

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6 Lake Ice cover – LIC

6.1 LIC validation activities

Lake ice cover (LIC) is a level 3 (L3) product generated from MODIS Terra/Aqua Level 1B calibrated radiances product (MOD02/MYD02), Collection 6.1 (TOA reflectance data) on a 250-m grid (at the Equator), then temporally (daily) and spatially aggregated onto the harmonized grid (1/120 degrees) of Lakes_cci. LIC product assessment is performed following three methods: (Method 1) validation against pixels extracted for a selection of lakes from visual interpretation of original MODIS Terra/Aqua imagery (RGB colour composites) used as input into the LIC retrieval algorithm; (Method 2) comparison with ground-based nearshore observations; and (Method 3) comparison with ice/open water extracted from the Interactive Multisensor Snow and Ice Mapping System (IMS) 1 km product (available since December 2014). A description of the methods and related inputs are described in Section 6.3 and foreseen challenges in Section 6.4.

6.2 Schedule for LIC validation

The table below provides an overview of the validation activities during Phase 2 (2022-2025) of Lakes_cci.

Validation activity	Time frame for analysis	Implementation
Algorithm calibration and uncertainty characterisation for MERIS	Completed in project phase 1 (2018-2022)	MERIS and OLCI (propagated) algorithms and pixel uncertainties in CRDP v1.0
<u>Method 1</u> : Validation of LIC CRDP v3.0 through visual interpretation of original MODIS Terra/Aqua imagery (RGB colour composites) used as input into the LIC retrieval algorithm.	September 2023 – July 2025	Random forest algorithm update with additional training data, processing chain update, and pixel-level uncertainties for CRDP v3.0
<u>Method 2</u> : Comparison with ground- based nearshore observations where match-up exists.		
<u>Method 3</u> : Comparison with ice/open water extracted from IMS 1 km product.		

Table 6-1 LIC validation schedule.

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6.3 Inputs and methods for LIC validation

Inputs for validation of the LIC product depend on the method selected. Each method and datasets for validation are described below.

Method 1: Validation against sets of pixels extracted for a selection of lakes from visual interpretation of MODIS TOA reflectance imagery

The Lakes_cci LIC product will be validated against ice, open water and clouds determined from the visual interpretation of MODIS Terra/Aqua Level 1B calibrated radiances product (MOD02/MYD02), Collection 6.1 (TOA reflectance data) – the primary product used as input in the LIC retrieval algorithm – during both



the freeze-up and break-up periods. Sets of pixels will be randomly chosen from a selection of lakes distributed globally to evaluate the LIC product. Both overall and class-specific accuracies will be reported.

Method 2: Comparison with ground-based nearshore observations

This method involves the comparison of ice/open water dates from a set of pixels of the Lakes_cci LIC product against those ground-based observations. Ground-based ice observations are made along lake shores, sometimes in bays, such that they can only be compared to one or a few satellite pixels located close to shore but far enough to be uncontaminated by land. The number of lake sites where ice observations are recorded coincident with satellite derived LIC product dates is likely to be small since there has been a drastic decline in such sites globally over the last three decades (Murfitt and Duguay, 2021). The ground-based observations will be extracted from the Global Lake and River Ice Phenology Database (GLRIPD; <u>https://nsidc.org/data/g01377/versions/1</u>) from the National Snow and Ice Data Center (NSIDC) (Benson et al., 2000, updated 2020).

Method 3: Comparison with ice/open water extracted from IMS 1 km product

The Lakes_cci LIC product will be compared to daily ice/water observations from the IMS 1 km gridded product (available since December 2014). IMS is a gap-filled product generated by the U.S. National Ice Center (2008) and available from NSIDC (<u>https://nsidc.org/data/g02156/versions/1#anchor-2</u>). A variety of multi-sourced datasets (e.g., AVHRR, GOES, SSMI, Ice Charts; for a complete list of data sources, see NSIDC, <u>https://nsidc.org/data/g02156</u>) are used by ice/snow analysts to produce maps that distinguish between land, snow-covered land, water, and ice. Analysis for ice cover relies primarily on AVHRR or MODIS imagery, however when visible imagery is not available, microwave-based retrievals and/or ice climatology are used (Helfrich et al. 2007). The 4 km version of the IMS dataset has been used to document variability and changes in LIC (2004-present) across the Northern Hemisphere (e.g. Duguay and Brown, 2018; Brown and Duguay, 2022).

With the IMS 1 km product it will be possible to compare ice-on and ice-off dates with those of the Lakes_cci LIC product. On cloud-free days it will also be feasible to compare LIC as per GCOS definition, which refers to the area of lakes covered by ice, expressed in km² (GCOS, 2022). LIC area will be computed from both products for a set of lakes to determine if the MODIS-derived Lakes_cci ice product achieves the GCOS minimum (threshold) required measurement uncertainty of 10%.

6.4 Known constraints for LIC validation

There are no foreseen constraints for the validation/cross-comparison of the Lakes_cci LIC product from Method 1 since this has been the primary approach relied upon at the very start of the project. Greater challenges are expected for assessment based on Method 2 and Method 3. First, in the case of Method 3, the IMS 1 km product is a "cloud-free" (gap-filled) product generated from ice/snow analysts who assign all grid cells in a lake as either ice or open water. Therefore, comparison will be made only for ice/open water matchups by focusing on clear days. In addition, the IMS product on a 1 km grid has only been produced since December 2014. Hence, the number of matchups may be low. Finally, the use of ground-based observations (Method 2) may be of limited use for evaluation of the Lakes_cci LIC product since observations are made close to shore while the MODIS-derived product provides ice/open water presence for some distance away from shore. Some discrepancies in ice dates are therefore expected due to the inherent nature of the products.

Validation and product uncertainties

As described in section 6.3, product validation activities are to include comparison against ground-based nearshore ice/open water observations (Method 2), the IMS 1 km product (Method 3), and validation against sets of pixels extracted from a selection of lakes from visual interpretation of MODIS RGB reflectance imagery (Method 1). The latter approach has been used internally to quantify total uncertainty



of the LIC product through computation of a confusion matrix built on an independent statistical validation. Classification error (%) derived from the confusion matrix is the metric used to report total uncertainty for each class (ice, water, cloud). Hence, in the case of LIC, there is a strong relation between validation activities and product uncertainty characterization.

The main sources of uncertainty of the LIC product are described in detail in E3UB. They have not been quantified independently. The identified sources include MODIS Aqua/Terra detectors noise/sensors degradation, observation noise (optical thickness of the atmosphere and view zenith angle/solar zenith angle), the threshold-based retrieval algorithm used, and misclassification. Evaluation of the LIC product by external users and activities under the consistency option will permit to identify in space (different lakes and lake sections) and in time (ice and open water seasons) where and when one or more of these sources of uncertainty are affecting the quality of the LIC product.

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7 Lake Ice Thickness- LIT

7.1 LIT validation activities

LIT validation activities involve:

- 1. The comparison of the LIT timeseries with the LIT obtained from thermodynamic model simulations, Canadian Lake Ice Model (CLIMo) (Duguay et al. 2003), and, for qualitative assessment only, with in-situ data, when available.
- 2. The comparison of the LIT estimates obtained from different altimetry missions during overlapping time periods, typically the tandem phases, for internal validation and consistency checks.
- 3. Consistency checks with MODIS and synthetic aperture radar (SAR) images for specific targets and periods, particularly during the shoulder seasons; during initial ice formation when the ice is thin and at the beginning of break-up with surface melt onset.
- 4. Cross-ECV consistency checks, typically with the LIC and LWST thematic products.

7.2 Schedule for LIT validation

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The validation of the LIT product with CLIMo simulations will be performed over the complete time span of the LIT timeseries before each product release. The validation and consistency of the LIT estimates obtained from different missions during overlapping periods will be performed before the merging of the intermediate products, generated for each mission, to the final product. The consistency assessment of the LIT estimates with MODIS and SAR images will be performed on chosen periods and targets. The comparison with in-situ data will be also performed during chosen periods and targets, according to availability. The cross-ECV consistency will follow the same schedule as for the other ECVs.

7.3 Inputs and methods for LIT validation

The inputs for LIT timeseries validation are the LIT timeseries generated with thermodynamic CLIMo simulations with different snow-on-ice scenarios. For qualitative cross-checks only, the in-situ LIT measurements will be used based on availability. In the case of the Great Slave Lake (target lake included in the CRDPV2.1) the in-situ data (up until April 28, 2016) are provided by the Canadian Ice Service (<u>CIS</u>). MODIS and SAR (Sentinel-1 and RADARSAT) images will also be used as input for consistency assessment.

Lake ice models are a valuable tool for the assessment of remote sensing-based ice thickness retrieval algorithms when in-situ measurements are absent or limited. Also, in-situ data are in general collected near the shore, therefore in a region of the lake far away from the satellite ground track from which the radar altimetry LIT estimates are achieved, making in-situ data not adequate to precisely validate the LIT from remote sensing. This is indeed the case for the Great Slave Lake, as the combination of differences in lake depth (10 m vs 30 m) and snow mass (depth and density) on the ice surface between the weather station and the satellites' tracks, precludes the use of the in-situ measurements for validation of the LIT estimates. The chosen lake ice model to validate the lakes_cci LIT timeseries is CLIMo (Duguay et al. 2003), a 1-D thermodynamic ice model, extensively used in the literature. The model can be forced using data from weather station observations, atmospheric reanalysis or climate model gridded products. The input (forcing) data consist of mean daily near-surface air temperature, relative humidity, wind speed, cloud cover, and snowfall (or snow depth from a nearby land site when available). A fixed mixed layer depth and typical (average) snow density must also be specified. The air temperature, cloud cover, relative



humidity, and wind speed are derived from the ERA5 atmospheric reanalysis product from the European Centre for Medium-Range Weather Forecasts (ECMWF). When not available from ERA5, the snowfall or snow depth data are derived from meteorological stations. In the case of the Great Slave Lake these data are collected at the Hay River weather station. To account for snow drifting on the lake ice surface, which is a process well documented in several studies on high-latitude lakes such as GSL, CLIMo is run with three sets of snow depth scenarios; 25, 50 and 75 % of the snow depth measured at the Hay River weather station and with a mean density of 300 kg m–3.

Another important consistency test is the comparison between the LIT estimates obtained from different satellites during the same period and, ideally, along the same track, that is, during the tandem phase between two satellites. This kind of test can be performed for instance when generating LIT timeseries with Jason missions, as it is the case of the CRDPv2.1. To quantitively compare the results, the Mean Bias Error (MBE) and the Root Mean Square Error (RMSE) can be computed between two LIT timeseries on the same dates during the overlapping periods.

Figure 10 from Mangilli et al. (2022) shows an example of the comparison of different LIT estimates over Great Slave Lake for the 2015-2016 winter season (WS3). The figure provides a comparison between LIT estimates with the LRM_LIT retracker from radar altimetry data, Jason-2 (triangles) and Jason-3 (stars) data, CLIMo simulations (diamonds) and in-situ data (circles). The shaded areas correspond to the LIT estimation uncertainties (at +/- 1 sigma around the LIT estimates), computed from Jason-2 data (blue) and Jason-3 data (red). Three different realizations of CLIMo simulations are shown by varying the amount of snow on the ice surface. The in-situ data consist of ice thickness measurements collected in Back Bay near Yellowknife. The agreement between Jason-2/3 LIT estimates and in-situ LIT data is only qualitative, showing a similar trend but higher LIT values with respect to the in-situ data, and ice formation occurring earlier in the season near the shores of GSL than in the middle of the lake. Table 7-1 summarizes the following indicators: the maximum of the LIT estimates, with the corresponding date, the mean LIT, the MBE and RMSE between the LIT estimates of Jason-2 and the other data sets.

Table 7-1 Comparison of the LIT results from rada	ar altimetry data and the CLIMo simulations
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$\left[\right]$	Season	Data	Δ^M_{ICE} [m]	$Date_{\Delta_{ICE}^{M}}$	$\mu_{\Delta_{ICE}}$ [m]	MBE [m]	RMSE [m]
Π	WS3	Jason-2	1.182 ± 0.091	18-04-16	0.994 ± 0.015	-	-
	WS3	Jason-3	1.208 ± 0.125	18-04-16	1.014 ± 0.012	0.013	0.024
	WS3	CLIMO-25	1.207	21-04-16	1.071 ± 0.007	-0.067	0.071
	WS3	CLIMO-50	1.171	26-04-16	0.999 ± 0.007	0.002	0.019
	WS3	CLIMO-70	1.114	26-04-16	0.949 ± 0.007	0.052	0.054

The agreement between the Jason-2 (blue triangles) and Jason-3 (red stars) LIT estimates is excellent (see the bottom panel of Figure 10). In the middle of the ice season, the MBE is only 0.013 m and the RMSE is 0.024 m between the two data sets. Also, the difference in the LIT mean value is only 0.02 m and that of maximum LIT is 0.025 m. Both Jason-2 and Jason-3 LIT are in strong agreement with the thermodynamics simulations with 50% of snow on ice as input (CLIMo-50 simulations), in particular in the middle of the ice season where the MBE between Jason-2 and CLIMo-50 is less than 0.01 m and the RMSE is 0.019 m. Overall, these representative results demonstrate that LIT estimates can be retrieved from radar altimetry data that are compatible with thermodynamic simulations and qualitatively in agreement with in-situ measurements.

Finally, the superposition of the LIT estimates on MODIS and SAR images will also be considered for better assessing the consistency of the LIT timeseries over specific periods, in particular at the seasonal transitions. SAR/optical images are in fact particularly useful for identifying deformation features (e.g., rafting), open leads in ice, and surface melt conditions (i.e. episodic and generalized melt during the break-up period) which are known to impact LIT retrievals from radar altimetry.





Figure 10 Comparison of LIT estimates over the Great Slave Lake for three winter seasons: 2013-2014 (top), 2014-2015 (middle), and 2015-2016 (bottom). From Mangilli et al. (2022).

7.4 Known constraints for LIT validation

Ground-based (in-situ) measurements will be used for qualitative comparison rather than validation of the LIT products. This is due to the fact that in-situ measurements of LIT are generally collected near the shore of lakes, while satellite data are chosen in the middle of the lake to avoid the impact of land contamination. These are indeed two different environments in terms of bathymetry, wind exposure, snow density and depth. All these parameters play a key role on ice formation and growth, and they can lead to LIT differences in the order of tens of centimetres, thus much bigger than the LIT retrieval accuracy, making in-situ data not always suitable for robust and precise validation of LIT products.

7.5 LIT references

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8 Conclusions

From CRDP v2.0.2 to v2.1 we will see an extension of existing products into 2021-2022, and additional quality criteria applied to LWLR as a result of product consistency investigations completed on v2.0.2. Otherwise, methodologies for the five ECV products included in v2.0.2 remain the same, and the validation plans reflect this continuity. A new entry in the v2.1 release is the LIT product which will be offered (by way of demonstration of future releases) for a single lake.

Towards v3.0, further improvements are expected, including addition of new sensors and their respective validation. Nevertheless, both the limitations to product validation (limited volumes of in-situ reference observations) remain largely the same as before, while growing time-series contribute to increased scope to assess overall product stability.

In addition to the per-product validation plans in this document, use cases and assessment reports contribute to pre-release validation of the Lakes ECV datasets. During the current project phase, use cases are particularly varied, ranging from the extraction of lake and regional trends within a climate dashboard intended for a wide audience including policymakers, to investigating the effects of heatwaves on lake biogeochemistry. These investigations are likely to prompt detailed investigations, particularly on inter-product consistency.



Appendix A - List of Acronyms

AATSR	Advanced Along Track Scanning Radiometer
AATSR	Advanced Along Track Scanning Radiometer
AERONET-OC	Aerosol Robotic NETwork – Ocean Color
AMI	Active Microwave Instrument
AMSR-E	Advanced Microwave Scanning Radiometer for EOS
APP	Alternating Polarization mode Precision
ASAR	Advanced Synthetic Aperture Radar
ASLO	Association for the Sciences of Limnology and Oceanography
ATBD	Algorithm Theoretical Basis Document
ATSR	Along Track Scanning Radiometer
AVHRR	Advanced very-high-resolution radiometer
BAMS	Bulletin of the American Meteorological Society
BC	Brockman Consult
C3S	Copernicus Climate Change Service
CCI	Climate Change Initiative
CDR	Climate Data Record
CDOM	Coloured Dissolved Organic Matter
CEDA	Centre for Environmental Data Archival
CEMS	Centre for Environmental Monitoring from Space
CEOS	Committee on Earth Observation Satellites
CGLOPS	Copernicus Global Land Operation Service
CIS	Canadian Ice Service
CLS	Collecte Localisation Satellite
CMEMS	Copernicus Marine Environment Monitoring Service
CMUG	Climate Modelling User Group
CNES	Centre national d'études spatiales
CNR	National Research Council of Italy
CORALS	Climate Oriented Record of Altimetry and Sea-Level
CPD	Communication Plan Document
CR	Cardinal Requirement
CRG	Climate Research Group
CSWG	Climate Science Working Group
СТОН	Center for Topographic studies of the Ocean and Hydrosphere
DOC	Dissolved Organic Carbon
DUE	Data User Element
ECMWF	European Centre for Medium-Range Weather Forecasts
ECV	Essential Climate Variable
ELLS-IAGRL	European Large Lakes Symposium-International Association for Great Lakes Research
ENVISAT	Environmental Satellite
EO	Earth Observation
EOMORES	Earth Observation-based Services for Monitoring and Reporting of Ecological Status
ERS	European Remote-Sensing Satellite
ESA	European Space Agency
ESRIN	European Space Research Institute
ETM+	Enhanced Thematic Mapper Plus
EU	European Union
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
FAQ	Frequently Asked Questions
FCDR	Fundamental Climate Data Record



FIDUCEO	Fidelity and Uncertainty in Climate data records from Earth Observations
FP7	Seventh Framework Programme
GAC	Global Area Coverage
GCOS	Global Climate Observing System
GEMS/Water	Global Environment Monitoring System for freshwater
GEO	Group on Earth Observations
GEWEX	Global Energy and Water Exchanges
GloboLakes	Global Observatory of Lake Responses to Environmental Change
GLOPS	Copernicus Global Land Service
GTN-H	Global Terrestrial Network – Hydrology
GTN-L	Global Terrestrial Network – Lakes
H2020	Horizon 2020
HYDROLARE	International Data Centre on Hydrology of Lakes and Reservoirs
ILEC	International Lake Environment Committee
INFORM	Index for Risk Management
IPCC	Intergovernmental Panel on Climate Change
ISC	International Science Council
ISO	International Organization for Standardization
ISRO	Indian Space Research Organisation
JRC	Joint Research Centre
KPI	Key Performance Indicators
LEGOS	Laboratoire d'Etudes en Géophysique et Océanographie Spatiales
LIC	Lake Ice Cover
LIT	Lake Ice Thickness
LSC	Lake Storage Change
LSWT	Lake Surface Water Temperature
LWE	Lake Water Extent
LWL	Lake Water Level
LWLR	Lake Water Leaving Reflectance
MERIS	MEdium Resolution Imaging Spectrometer
MGDR	Merged Geophysical Data Record
MODIS	Moderate Resolution Imaging Spectroradiometer
MSI	MultiSpectral Instrument
MSS	MultiSpectral Scanner
NASA	National Aeronautics and Space Administration
NERC	Natural Environment Research Council
NetCDF	Network Common Data Form
NOAA	National Oceanic and Atmospheric Administration
NSERC	Natural Sciences and Engineering Research Council
NSIDC	National Snow & Ice Data Center
NTU	Nephelometric Turbidity Unit
NWP	Numerical Weather Prediction
OLCI	Ocean and Land Colour Instrument
OLI	Operational Land Imager
OSTST	Ocean Surface Topography Science Team
PML	Plymouth Marine Laboratory
PP	Payment Plan
PRISMA	PRecursore IperSpettrale della Missione Applicativa
Proba	Project for On-Board Autonomy
QSR	Quarterly Status Report
R	Linear Correlation Coefficient
RA	Radar Altimeter
RMSE	Root Mean Square Error



SAF	Satellite Application Facility
SAR	Synthetic Aperture Radar
SeaWIFS	Sea-viewing Wide Field-of-view Sensor
SIL	International Society of Limnology
SLSTR	Sea and Land Surface Temperature Radiometer
SoW	Statement of Work
SPONGE	SPaceborne Observations to Nourish the GEMS
SRD	System Requirements Document
SSD	System Specification Document
SST	Sea Surface Temperature
STSE	Support To Science Element
SWOT	Surface Water and Ocean Topography
TAPAS	Tools for Assessment and Planning of Aquaculture Sustainability
ТВ	Brightness Temperature
TM	Thematic Mapper
TOA	Top Of Atmosphere
TR	Technical Requirement
UNEP	United Nations Environment Programme
UoR	University of Reading
UoS	University of Stirling
US	United States
VIIRS	Visible Infrared Imaging Radiometer Suite
WCRP	World Climate Research Program
WHYCOS	World Hydrological Cycle Observing Systems
WMO	World Meteorological Organization
WP	Work Package

