FLEX DISC

FLUORESCENCE EXPLORER DATA INNOVATION AND SCIENCE CLUSTER

L2C CALIBRATION/VALIDATION PLAN

Document Information

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1. Introduction

1.1 Scope of the document

The scope of this document is to provide all the information needed to define the validation plan for FLEX L2C products. Currently, the driving requirements are described in the FLEX Mission Requirements Document (MRD). In this document, we present the strategy to evaluate FLEX L2C products. Indications presented in this report are needed for preparing the FLEX Validation Plan, which is planned as a living document and still in preparation and updated in time.

In this document and elsewhere we use the term "L2 product" to refer to the Level 2 physical product as described in the L1C & L2 IPF Product Format Definition [RD-20]. The L2 product contains three logical products as follows (see [RD-20]):

- L2A: the group of L2 Atmospheric products,
- L2B: the group of L2 Fluorescence products, and
- L2C: the group of L2 Vegetation products.

Hereafter, we use the terms "L2A Product", "L2B Product", and "L2C Product" to refer to the corresponding group of parameters in the L2 Product.

Similar documents will be prepared according to the structure defined in the FLEX Cal/Val plan overview. The validation plan of FLEX is in fact made of different components, organized to provide a useful roadmap for evaluating the overall quality of the mission's core products. Overall, FLEX Validation activities, for each product, should address four main objectives, which can be reached at different times of the mission:

a) to develop and prepare documentation, guidelines, and tools for validation of products before the Commissioning Phase;

b) to provide a comprehensive initial assessment of product validity and quality of the FLEX core products at the end of commissioning activities;

c) to monitor the stability and the quality of the products throughout the operational phase of the mission;

d) to continuously improve the quality of the products throughout the operational phase of the mission, following the evolving user requirements.

This specific implementation plan is intended to present the actual tasks and activities that will be performed to address the requirements about how the validation work for L2C products shall be done.

While chapter 1 of this document provides information about related documents, in chapter 2 definitions of the traditional and advanced biophysical variables are provided. Chapter 3 gives an overview about the validation procedures that are planned to be used for the different L2C products. The first part of the chapter is focussed on the direct validation and the second part describes the planned approaches for the indirect validation. The document is concluded describing the planned activities within the L2C product validation during the pre-launch, commissioning and operational phase of FLEX.

1.2 Related documents

1.1.1 Applicable documents

Id.	Ref.	Description	Issue
[AD-01]	ESAEOP-SM/2221/MDru-md	FLEX EE8 Mission Requirements Document	3.0
[AD-02]	FLX-TN-ESA-SYS-0032	FLEX Mission Architecture and Operations Concept	2.0
[AD-03]	FLX-ADD-GMV-FIPS-GPP	FLEX L2 E2E Mission Performance Assessment - Architecture Design Document	2.2.2
[AD-04]	FLX-ICD-GMV-FIPS-GPP	FLEX L2 E2E Mission Performance Assessment - Interfaces Control Document	2.2.3
[AD-05]	ESA-EOPG-PR-0005	EOP-G Security operating procedure (SECOPS) framework	1.0
[AD-06]	GMGT-SENE-EOPG-PD-12-0011	EOP-G Security Incident Handling Policy	1.1
[AD-07]	ESA-EOPG-EOEP-DD-0003	FLEX PDGS System Architecture Document	2.5
[AD-08]	ESA-EOPG-EEGS-ID-0083	Generic Processor ICD	1.4
[AD-09]	ESA-EOPG-EOEP-ID-0009	FLEX PDGS CPF-IPF Interface Control Document	1.4
[AD-10]	ESA-EOPG-EOEP-TN-0015	FLEX PDGS Products Naming Convention and Definition	2.12
[AD-11]	ESA-EOPG-EOEP-TN-0025	FLEX PDGS Main Product Header Definition	1.5
[AD-12]	ESA-EOPG-EOEP-TN-0014	FLEX PDGS Production Model	1.1
[AD-14]	ESA-EOPG-EOPGMQ-SOW-43	FLEX DISC Statement Of Work	1.0

1.1.2 Reference documents

Id.	Ref.	Description	Issue
[RD-01]	EOP-SM-3044-MDru-mdru	FLEX Mission Product Tree & Product Definition	2.0
[RD-02]	EOP-SM/2776	Scientific Readiness Levels (SRL) Handbook	1.1
[RD-03]	FLX-LI-ESA-SYS-0017	FLEX Acronyms, Terms and Definitions (ATD)	1.3
[RD-04]	ECSS-E-HB-40-01A	Agile software development handbook	1.0
[RD-05]	ESA-EOPG-EOEP-TN-0013	FLEX PDGS Product Baseline Definition and Usage	1.0
[RD-06]	ESA-EOPG-EOEP-TN-0026	FLEX PDGS Auxiliary Product Format Definition	2.1
[RD-07]	ESA-EOPG-EOEP-TN-0027	FLEX PDGS RAW Products Format Definition	2.9
[RD-08]	ESA-EOPG-EOEP-TN-0022	FLEX PDGS Level-0 Product Format Definition	2.6
[RD-09]	ESA-ESO-PR-2020-0039	Instructions Regarding the Common Protection of Unclassified Programme/Project Information	2.0
[RD-10]	ISO/IEC 15408D	Common Criteria for Information Technology Security Evaluation	
[RD-11]	FLX-RS-ESA-GS-0043	FLEX Ground Segment Requirements Document (GSRD)	2.1
[RD-12]	MAG-23-PTF-86-Vol1	FLEX DISC Technical Proposal	2.1
[RD-19]	FLEXDISC-PMP-MAG-002	FLEX DISC Project Management Plan	1.1
[RD-20]	FLEXDISC-IPF-PFD-MAG-016	L1C & L2 IPF Product Format Definition	1.4

1.1.3 Other related documents

Id.	Ref.	Description	Issue
[OD-01]	FLEXDISC-CALVAL-PLAN-UMB-030	FLEX DISC Cal/Val Plan Overview	0.2
[OD-02]	FLEXDISC-CALVAL-PLAN-UMB-060	L2B Validation Plan	0.1

1.1.4 Definitions and Acronyms

The FLEX Acronyms, Terms and Definitions are listed in [RD-03]. Additional definitions and acronyms not covered in [RD-03] are listed below.

CP Collaborative Platform

DHP Digital hemispherical photography

ESL	Expert Support Laboratory
LAI	Leaf area index
APAR	Absorbed photosynthetically active radiation
fAPAR	Fraction of absorbed photosynthetically active radiation
RED	Regulated energy dissipation
FVC	Fractional vegetation cover
ETR	Electron transport rate
FQE	Fluorescence quantum efficiency
L2RM	Level 2 retrieval module
L2PP	L2 processor prototype
SCOPE	Soil Canopy Observation, Photochemistry and Energy fluxes model

2. L2C product description

2.1 Traditional biophysical variables

2.1.1 Leaf Area Index - LAI

Leaf Area Index (LAI) is defined as the total one-sided area of all leaves per unit ground area in the canopy within a defined region, and is a non-dimensional quantity, although units of m^2 m^{-2} are often used. The Gaussian process regression (GPR) processor that is used in the L2RM uses a 1D radiative transfer model to generate the training data set, and hence it models effective LAI (uncorrected for the well-known clumping effects, which may lead to underestimated values particularly in forests). For the correction of clumping, no universally accepted method exists. For the mentioned applications (interpretation of SIF and the future estimation of GPP), the effective LAI may suffice as it can be used in Beer-Lambert models.

2.1.2 Leaf chlorophyll content - LCC

Leaf chlorophyll content (LCC, µg m^{-2}) is currently further used in the L2RM to calculate the CO_2 flux. However, the CO_2 flux is not part of the product handbook (REF1), see later in this document, and hence, LCC is not required to further compute the L2C products. Nevertheless, LCC can be of interest to users, who may be interested in the chlorophyll content in conjunction with SIF. Furthermore, it is possible to validate LCC with some limitations. It should be clarified that the retrieved LCC is an effective value for the pixel footprint, and due to the heterogeneity and non-linearity this may be different (typically lower) than the numerical average of all leaves (which can be in the order of 10^7 to 10^9 leaves per pixel footprint).

2.1.3 Fraction of Absorbed Photosynthetically Active Radiation - fAPAR

The Fraction of Absorbed Photosynthetically Active Radiation (fAPAR) is defined as the fraction of Photosynthetically Active Radiation (PAR; solar radiation reaching the surface in the 400-700 nm spectral region) that is absorbed by a vegetation canopy. fAPAR can be defined as a photon ratio, or an energy ratio. The fAPAR is defined at the level of the stand (the pixel footprint) and it is sensitive to both the leaf density (LAI) and the absorption by leaves. For the users, who may want to use the product in light use efficiency models, the photon ratio is most useful. Furthermore, 'white sky' (only diffuse illumination), 'black sky' (only direct illumination) and 'blue sky' (mixed illumination) fAPAR may be differentiated. The 'white sky' fAPAR is a pure vegetation characteristic, and is insensitive to the illumination geometry. The 'blue sky' value is sensitive to the illumination geometry, and hence it exhibits a diurnal cycle, but it may be more useful for the interpretation of SIF than white sky fAPAR because it represents the fAPAR at the FLEX overpass time. The blue sky fAPAR can be validated during overpass time by PAR measurements in the field. The white sky fAPAR can only be validated indirectly from the blue sky value by some radiative transfer computations, or measured during cloudy conditions close to the day of the overpass The blue sky fAPAR in units of photons m-2 s-1 will be provided as L2C product. Absorbed Photosynthetically Active Radiation - (APAR, photons m^{-2} s^{-1}) can be calculated by the user as the fAPAR and iPAR, where iPAR is the incident irradiance.

2.2 Advanced biophysical variables

2.2.1 Absorbed Photosynthetically Active Radiation by chlorophyll ab (APAR_ch)

Absorbed Photosynthetically Active Radiation by chlorophyll ab (APAR_ch) is the share of blue sky APAR that is solely being absorbed by chlorophyll a and b pigments. APAR_chl will be provided in photon units (photons m^{-2} s^{-1}).

2.2.2 Leaf carotenoid content - LCARC

The total carotenoid content (LCAR) plays an important role in photosynthesis and phenology studies and will be provided in µg cm^{-2}. The retrieval is nearly identical to that of LCC, and it is possible to validate LCARC.

2.2.3 Fluorescence quantum yield - FQE

The quantum yield of fluorescence (FQE) is defined as the probability that a photon of VIS radiation (400—700 nm) absorbed by chlorophyll is dissipated as a fluorescence photon (650-850 nm). The product is defined as the effective value at the stand (pixel footprint) level, as the ratio of the emitted fluorescence (spectrally and hemispherically integrated and corrected for (re-)absorption) over aPAR_chl. In the scientific literature FQE at the leaf level is also referred to as fluorescence yield (PhiF) in ambient light conditions (a state called 'Fs' in the active fluorescence literature). The absolute value of FQE can be accurately measured with time-resolved fluorescence spectroscopy, using an excitation laser diode pointing at an individual leaf. If the FQE of individual leaves is measured, then a scaling exercise is required to obtain a canopy effective value that is comparable to the satellite data product. Alternatively, FQE at the stand level can be obtained by applying a similar retrieval algorithm as used in the L2C processor, but using field measurements of SIF as input. Finally, relative measurements of FQE on individual leaves can be obtained by using a calibrated PAM instrument, where the fluorescence is induced by a measurement light.

2.2.4 Proxy of regulated heat dissipation - RED

Regulated energy dissipation (RED) refers to the energy released by the collective reversible mechanisms (processes) of the plant to protect itself from the adverse consequences of excess illumination. It is the product of the absorbed photosynthetically active radiation, and the probability that this absorbed radiation is dissipated as heat through these processes (the so-called yield). RED can be defined in energy flux or in photon flux. In order to facilitate the comparison to ETR and to make the validation easier, the photon flux unit is adopted here. Thus, RED is phiN*aPARchl. The yield phiN is calculated by means of rate coefficients, as $Phi_n = K_n/(K_f + K_d + K_p + K_n)$, where Kn, Kp and (Kd+Kf) can all be computed from measurements with active fluorescence instruments in the field, notably the measurements Fm, Fm', Fo, Ft. Fm (Fm') is the fluorescence of a dark (light) adapted leaf induced by a weak, oscillating measurement light during a saturating flash, Fo the fluorescence of a leaf in response to a weak, oscillating measurement during nocturnal darkness, and Ft the steady-state fluorescence in response to a weak oscillating measurement light during the day.

The FLEX L2C product refers to the fraction of absorbed photons (photons m^{-2} s^{-1}) that is emitted as variable heat dissipation. Multiplication by $fAPAR_{chl}$ and integration over leaves to the stand level then results in the RED rate (photon m^{-2} s^{-1}) comparable to

the L2C product. Alternatively, RED obtained from PAM fluorometry can be converted to a RED-yield (phiN) and scaled to the stand level.

2.2.5 Electron transport rate - ETR

The electron transport rate (ETR) is the rate by which excited electrons reach the reaction centers of photosystems. The L2C product is defined at the stand (pixel footprint) level, as the product of the photochemical yield (phiP) and fAPAR_chl. Initially the L2C product will comprise a light-use efficiency model estimate based on APAR_Chl, LST and FQE, and depending on the success of NPQ retrieval, this will be later refined. At leaf level, ETR can be estimated as the product of PhiP obtained from PAM fluorometry and fAPAR_chl. An absolute value of PhiP can be obtained from PAM without the need for time-resolved fluorescence measurements. Scaling of the measurements from the leaf to the whole stand (integration) is required to convert a leaf level measurement of ETR (electrons m^{-2} leaf s^{-1}) to the stand (electrons m^{-2} s^{-1}) is necessary to obtain a quantity comparable to the L2C product.

2.2.6 Fluorescence escape fraction – fesc

The escape probability, also referred to as the fluorescence scattering function sigmaF in the scientific literature, is defined as the ratio of TOC fluorescence radiance in observation direction times pi, divided by the fluorescence irradiance produced in the canopy by chlorophyll (SIF_RC). fesc has a smooth spectral shape that is similar, but not identical to the reflectance. It is provided as a spectrally resolved product, in a similar manner as the full spectrum of fluorescence (nodes that can be used to reconstruct the full spectrum). fesc cannot be directly validated in the field, but it can be compared to equivalents derived from field spectroscopy measurements with an algorithm similar to the L2C processor.

2.3. Mission Calibration and Validation requirements for each target variable

Since there are no mission requirements defined for the FLEX L2C variables, uncertainty ranges provided in literature will be used as reference and are provided below (Table 1).

Table 1 - Overall range of uncertainties. Variable units: LAI in m^2 m^{-2}, fAPAR is unitless, LCC in $\mu g\, cm^{-2}$.

	median accuracy indicators					
variables	**uncertainty range**	**R2**	**RMSE**	**MAE**	**known variable range**	**source**

LAI	7-20%. target: max(0.05, 10%) [1]	0.62	0.88	<0.1	0-10	Fang et al., (2019) GCOS (2016)
LCC			5.71 to 14.94 [2]	not availabl e	8 to 15 [3]	Croft et al., (2020) Houborg et al., (2015)
fAPAR	max(0.05, 10%) [4]				0-1 [5]	Copernicus Climate Change Service, Climate Data Store, (2018)
APAR_ch	<10%					AD-01
LCARC	not available					
FQE	not available					
RED	20-30%					AD-01
ETR	not available					
fesc	not available					

[1] GCOS (2016)
[2] Croft et al., (2020)
[3] Houborg et al., (2015)
[4] GCOS (2016)
[5] maximum value is never observed in practice

3. Validation Procedures

Multiple validation procedures will be carried out, while the choice of a specific validation procedure depends on the target variable. Overall, three different validation approaches will be applied: direct, indirect and cross-evaluation.

Direct validation refers to a set of approaches involving the comparison of satellite-derived products with independent in situ reference measurements. Direct validation will be carried out depending on the target variable and the availability of field measurements from field campaigns or networks providing biophysical data.

We define indirect validation as the comparison of satellite-derived target variables with proxy data sources or variables estimated through other models or algorithms. The indirect validation approach will be carried out by comparing L2C estimates from the L2RM algorithm with results from a model tuned to field or satellite data. This is unavoidable due to scale mismatches between the field and L2C data products. The SCOPE model will serve as the main vehicle for this purpose. SCOPE will be constrained by the locally available field and satellite information in order to scale the direct measurements to the FLEX pixel footprint. Depending on the specific local situation at the validation site, other models may be used as well for the scaling. Apart from the issue of scaling, indirect validation is also required for data products that cannot be directly observed, such as fAPAR_chl and fesc.

Cross-evaluation involves comparing the target variable obtained from one satellite mission with equivalent data products derived from other satellite missions. This method leverages the availability of multiple satellite datasets to evaluate the consistency, reliability, and accuracy of the satellite products under investigation.

3.1. Direct validation

3.1.1. Traditional biophysical variables

3.1.1.1 Specific Objectives

The objective is to collect in situ measurements of the target variables LAI, fAPAR and LCC to assess the quality of the FLEX LAI, LCC and fAPAR products retrieved with the L2C processor. For the validation of the three variables we suggest to follow the guidelines developed within the ESA project 'Fiducial Reference Measurements for Vegetation' (FRM4VEG). The FRM4VEG guidelines are published in the form of two reports that can be downloaded directly from the project website (https://frm4veg.org/documents/).

3.1.1.2 Description and justification of the methodology

In situ methods for measuring LAI and LCC can be distinguished in destructive (harvesting) and non-destructive (non-harvesting) methods. While destructive methods

enable LAI and LCC determination in a direct way, non-destructive assessment is based on the 'indirect' derivation of LAI and LCC from more easily measurable parameters. Since the validation of the LAI and LCC FLEX products, having a spatial resolution of 300 x 300 m, is labor, cost and time intensive, we propose to use non-destructive indirect techniques to collect a high number of LAI and LCC measurements close to the time of a FLEX overflight. However, due to the fact that LAI and LCC are not rapidly changing within a few hours up to a few days under normal conditions, LAI and LCC field measurements used for validation can be collected within a period of two days before to two days after a FLEX data acquisition, which makes the in situ data collection of the two parameters more practical and allows to collect a high number of reference data for the validation of the corresponding FLEX products.
In contrast, fAPAR can only be measured indirectly on the ground and has a mild solar illumination angle dependence, which affects the distribution of direct and diffuse illumination. The blue sky measurement at the time of overpass is directly comparable to the satellite data products, while measurements at other times of the day and under different weather conditions can be used as indirect validation after some geometrical correction and using models.

LAI
Several optical non-destructive methods have been developed in recent years, which require no physical contact with the leaves. Using these methods, the LAI can be indirectly derived from measurements of light transmission through the canopy in the field.
Digital hemispherical photography (DHP) is one of the non-destructive techniques to measure LAI on the ground. A fisheye lens mounted on an upward-pointing digital camera is used to acquire photos from beneath the canopy. The subsequent analysis of the photos with appropriate image processing software enables the assessment of the gap size distribution (exploiting the contrast between leaves and sky) and the determination of the LAI. Although DHP can be used for almost all types of canopies, this technique is mainly applied in forestry, where the assessment of incoming radiation above the canopy is difficult to measure.
In contrast, in agricultural ecosystems, which are characterized by low and regular canopies, the LAI is often calculated with devices that simply compare measurements of incoming light above and below the canopy. Different commercial devices are available, which measure the fraction of transmitted radiation that passes through a plant canopy. They all work on the same principle. The smaller the amount of radiation transmitted by the leaves, the higher is the LAI, and vice versa.
Due to the fact that hemispherical photography is the standard method to collect in situ LAI measurement in forest science, we propose to use this technique for the validation of the FLEX LAI product derived from forest ecosystems. For the validation of agricultural ecosystems and ecosystems characterized by low vegetation (e.g. shrublands) we propose to use light ceptometers, such as the Sunscan (Delta-T Devices Ltd, UK) or the AccuPAR LP-80 (Metergroup, USA), since both devices offer the

possibility to collect reliable LAI in situ measurements under diffuse and direct illumination conditions. As an alternative the LAI-2200C Plant Canopy Analyser (and previous LAI-2200 and LAI-2000 variants) (LI-COR Inc., USA) can also be used to indirectly collect in situ LAI measurements but only under cloudy conditions and timely close to the FLEX data acquisition. The instrument uses a fisheye optical sensor combined with an optical filter to accurately measure LAI.

LCC

Chlorophyll a and b (Chl_a and Chl_b) are the key photosynthetic pigments within a plant and thus determining LCC plays an important role in determining a plant's physiological status. The most widely used instrument to non-destructively measure relative LCC of plant leaves is the SPAD-502 chlorophyll meter (Konica-Minolta, Japan). The instrument can be used for different plant types in a variety of environmental conditions, and its measurement area of 2 x 3 mm enables even small leaves to be measured. Numerous scientific publications exist providing empirical equations for different plant types and growth stages that can be applied to transform the relative SPAD-502 readings into LCC in physical units (µg cm^{-2}). This is a decisive step to make the in situ measurements usable for the validation of the FLEX LCC product. Besides the SPAD-502 other handheld instruments using a similar measurement technique are available such as the PlantPen (Photon System Instruments, Czech Republic) or the MultispeQ (PhotoSynQ, USA).

fAPAR

The most efficient ways to collect a large number of in situ fAPAR measurements are to use quantum sensors, or to estimate it from measurements of transmission or gap fraction. Quantum sensors consist of a detector and filter that is sensitive to the PAR region of the electromagnetic spectrum, and typically incorporate cosine correction to provide a measurement integrated over the entire hemisphere. When measured directly, the PAR absorbed by a canopy is determined based on a closure of the PAR balance, considering hemispherical fluxes at the boundaries of the canopy.

A number of individual sensors are available commercially, with a range of performances in terms of spectral sensitivity, cosine response, and price. Examples include the LI-190R (LI-COR Inc., USA), SQ-100 series (Apogee Instruments Inc., USA), QS5 (Delta-T Devices Ltd, UK), and SP Lite 2 (OTT HydroMet B.V., The Netherlands).

Several manufacturers also provide a number of sensors aligned on a single support, enabling spatial variability in incoming PAR at the bottom of the canopy to be better represented. Such systems are known as ceptometers and can incorporate up to 80 individual sensors along a 1 m rod. Examples include the AccuPAR LP-80 (Metergroup, USA) and SunScan (Delta-T Devices Ltd, UK).

In addition, fAPAR can be derived from canopy transmittance/gap fraction at multiple zenith angles. The LAI-2200C Plant Canopy Analyser (and previous LAI-2200 and LAI-2000 variants) (LI-COR Inc., USA) makes use of an optical sensor to measure incoming radiation in the blue region of the electromagnetic spectrum. Measurements are performed both above and below the canopy, enabling canopy transmittance to be

determined. Since gap fraction can be considered nearly equal to canopy transmittance in the PAR domain, the angular variation in canopy transmittance/gap fraction can be used to reconstruct diurnal variations in the fraction of intercepted PAR (fIPAR), which can then be used to determine fAPAR.

3.1.1.3 Data requirements

Below the auxiliary data required for the L2C traditional biophysical parameter validation are listed:

i. geolocation information to account for accurate spatial comparison between in situ measurements and corresponding FLEX pixels
ii. land use/cover information to develop an appropriate spatial sampling strategy that provides information on the heterogeneity of the sampling area
iii. topographic information in the form of digital elevation models to take into account effects caused by differences in elevation and slope
iv. Sentinel-2 L1C or L2A satellite images at 10/20 m spatial resolution covering the locations of the in situ measurements are required for the upscaling of the in situ data (using the two-stage approach) to the spatial resolution of FLEX
v. potential in situ data for the validation of LAI and fAPAR from available direct validation networks and projects, such as BigFoot, SAFARI-2000, VALERI, ImagineS, OLIVE DIRECT 2.0 and GBOV

3.1.1.3 Data availability

Most of the networks and projects providing in situ reference data for the direct validation of LAI, LCC and fAPAR (listed in chapter 3.1.1.4) have only data available that were collected during field campaigns at specific field sites in the past. Some of the networks and projects are still running and future field campaigns are planned. The in situ measurements collected during those future campaigns can potentially be used to validate LAI, LCC and fAPAR products derived from FLEX in the commissioning or later in the operational phase. However, it is uncertain which sites will be sampled by the networks in the future, if FLEX data of the sites will be recorded timely close to the field campaigns, and if the sites and the applied sampling strategies are suitable for the validation of the FLEX products.

The most comprehensive collection of LAI and fAPAR ground-based observations is collected by the GBOV service and available free-of-charge on their website. The main advantage of GBOV is that their database includes in-situ LAI and fAPAR measurements collected over a series of selected sites organized through international research networks such as NEON, TERN and ICOS. For this reason, it has great potential for the validation of FLEX derived LAI and fAPAR products and will serve as an input data source for the LAI and fAPAR validation tools described in section 3.1.1.4.

However, taking into account the spatial coverage and revisit rate of FLEX, a proper validation of the different traditional biophysical L2C products, especially in the

commissioning phase, can only be ensured by conducting field campaigns adapted to FLEX. Since those field campaigns will be indispensable for the validation of the novel photosynthesis related variables (cf. section 3.1.2), LAI, LCC and fAPAR can additionally be measured during those activities.

3.1.1.4 Algorithm description

Two different solutions (approaches) will be used for the direct validation of the traditional biophysical variables. Following solution 1 LAI, LCC or fAPAR measurements collected in 20 x 20 m elementary sampling units (ESUs) distributed within a 3 x 3 km area are upscaled, to be representative for a FLEX pixel. The spatial upscaling is done by establishing a linear relationship between the mean value of the in situ measurements within the ESUs and vegetation index values derived from spatial high-resolution Sentinel-2 L1C or L2A data at the same locations recorded timely close to the field data acquisition. The following vegetation indices, which were identified sensitive to the target variable in different scientific publications, will be used:

Table 1: Vegetation indices used within the two stage approach for the spatial upscaling of LAI, fAPAR and LCC.

Parameter	**Vegetation index**	**Calculation from S-2**	**Literature**
LAI	Enhanced Vegetation index 2 (EVI2)	EVI2 = 2.5 * (B08 - B04) / (B08 + 2.4 * B04 + 1.0)	Jiang et al. 2008
fAPAR	Wide dynamic range vegetation index (WDRVI)	WDRVI = (0.1 * B08 - B04) / (0.1 * B08 + B04)	Gitelson et al. 2004, Vina and Gitelson, 2005
LCC	Chlorophyll Vegetation Index (CVI)	CVI = B08 * B04 / (B03)^2	Vincini et al. 2008

Determining the linear relationship (in the form of a linear regression model) between a traditional L2C variable and the respective index allows one to apply the 'two-stage' (also called 'bottom-up') approach proposed by the CEOS WGCV LPV sub-group. The determined linear regression models for the different variables can be applied to all Sentinel-2 pixels within the 3 x 3 km to generate spatial-high resolution LAI, fAPAR and LCC maps. Subsequently, the high resolution maps are aggregated to 300 m spatial resolution and resampled to match the locations of corresponding FLEX pixels. After conducting the aforementioned steps the matchup can be done using different validation metrics. The developed validation tools have the following names:

- LAI - *L2 LAI Val Campaign*

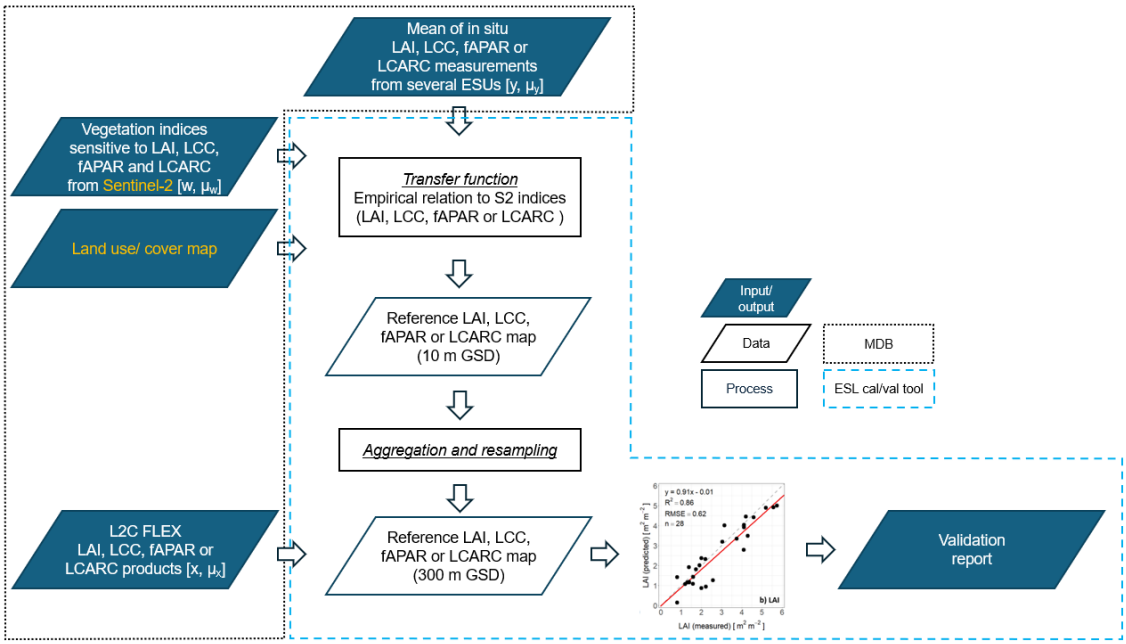
- fAPAR - *L2 fAPAR Val Campaign*
- LCC - *L2 LCC Val Campaign*

Solution 2 is based on in situ LAI and fAPAR data provided by the GBOV service that includes data collected by different biophysical networks at different locations around the globe (most locations are in Europe, the US and Australia). In contrast to validation solution 1 this software tool is using FLEX LAI or fAPAR maps recorded at different locations at different times for which corresponding in situ measurements from the different networks are available. Similar to solution 1 vegetation indices sensitive to LAI (EVI2) and fAPA (WDRVI) are calculated from Sentinel-2 L1C or L2A data for all pixels in a 30 m buffer around the in situ data measurement location recorded timely close to the ground observations and the FLEX data acquisition. The transfer (linear regression) function determined from the averaged index values within the 30 m buffer areas around the in situ measurement locations is then applied to the Sentinel-2 data covering an area of 1 x 1 km around the in situ measurement location to generate spatial high-resolution LAI and fAPAR maps. Those maps are then aggregated to 300 m spatial resolution and resampled to match the pixel locations of the corresponding FLEX product. As the final step the determined matchup pairs from different geographic locations can be compared to calculate the validation metrics. The developed validation tools have the following names:

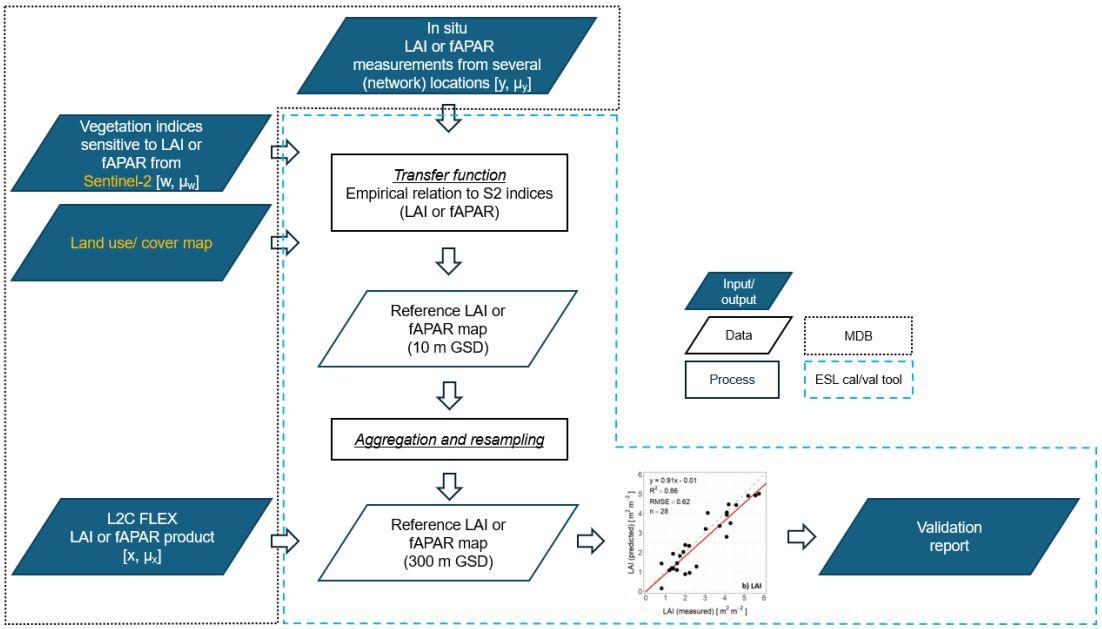
- LAI - *L2 LAI Val Network*
- fAPAR - *L2 fAPAR Val Network*

i. Cal/Val algorithm overview and algorithm flowchart

Solution 1 - *Multiple location measurements covering a small area (3 x 3 km) sampled in a field campaign*



Solution 2 - *Multiple location measurements around the globe sampled by different international research networks*



ii. Steps involved in reading and ingesting data (description)

Validation software - Solution 1

1. Input: Reading a text file containing averaged in situ measurements of the traditional biophysical variable in different ESUs, corresponding uncertainties, and x and y coordinates (UTM format) of the measurement locations.
2. Calculation of vegetation index sensitive to the target variable from 10 m spatial resolution Sentinel-2 data and determination of transfer (linear regression) function.
3. Applying transfer function to the Sentinel-2 data covering the 3 x 3 km area and aggregation of the target variable map to 300 m spatial resolution.
4. Comparison of the upscaled Sentinel-2 map with the pixel values of the corresponding FLEX L2C product using different validation metrics (e.g., R^2, RMSE, Std, Bias).
5. Output: Generating validation report providing validation metrics and visualization of the validation results in the form of scatter plots.

Validation software - Solution 2

1. Input: Reading csv file containing in situ LAI or fAPAR measurements from different network locations with corresponding x and y coordinates (UTM format).
2. Quality control of the the traditional biophysical variable in situ measurements

3. Calculation of vegetation index sensitive to the target variable from 10 m spatial resolution Sentinel-2 data in an area of 30 m around in situ sampling location and determination of the transfer (linear regression) function.
4. Applying transfer function to the Sentinel-2 data covering a 1 x 1 km area around in situ sampling location and aggregation of the target variable map to 300 m spatial resolution.
5. Comparison of the upscaled Sentinel-2 map with the pixel values of the corresponding FLEX L2C product using different validation metrics (e.g., R^2, RMSE, Std, Bias).
6. Output: Generating validation report providing validation metrics and visualization of the validation results in the form of scatter plots.

iii. Quality checks needed on the reference and auxiliary data

Prior to upscaling, quality control should be carried out to screen both in situ measurements and high spatial resolution S2 imagery for poor quality data. In the case of the high spatial resolution imagery, the quality flags provided with the product should be used to discard pixels contaminated by radiometric saturation or cloud cover. In the case of the in situ measurements, any measurement with a value of greater than two standard deviations from the mean should be examined to assess its validity. If the measurement is determined to be spurious, it should be discarded prior to further analysis.

iv. Colocation procedures to create match-up pairs including aggregation and transfer functions used to upscale

Collocation procedures for comparing in situ reference data and FLEX products are carried out as follows:

Temporal alignment: Due to the fact that LAI and LCC are not rapidly changing within a few hours up to a few days under normal conditions, LAI and LCC in situ measurements used for validation purposes can be collected within a period of two days before to two days after a FLEX data acquisition, which makes the in situ data collection of the two parameters more practical and allows to collect a high number of reference data for the validation of the corresponding FLEX products.
In contrast, fAPAR has a slight dependence on the angular position of the sun and the relative contributions of the direct and diffuse illumination. The blue sky in situ measurements at the time of the FLEX overpass are directly comparable to the satellite data products, while measurements at other times of the day and under different weather conditions can be used as indirect validation after some geometrical correction and using specific models.

Spatial alignment: Both validation solutions using the two-stage (bottom-up) approach that includes using spatially higher resolved Sentinel-2 data. For this reason, the x and y coordinates of the in situ sampling locations must be accurately measured by RTK

GPS devices. While this can be taken as granted by international research networks (solution 2), for field campaigns this is an additional but necessary effort (solution 1).

v. Comparison metrics and expected output/report

Error evaluation will consist of accuracy, precision and uncertainty evaluated by several metrics reporting the goodness of fit between the FLEX traditional biophysical products and the corresponding in situ reference dataset. Commonly, accuracy represents systematic errors while precision represents the dispersion of product retrievals around their expected value. Metrics of accuracy and precision are often computed as the statistical mean bias, standard deviation (Std), Root Mean Square Error (RMSE), and the linear regression (R^2) of the difference between L2C from satellite products and the corresponding reference estimates. Besides standard scatter plots providing information about the goodness-of-fit of in situ and satellite data (e.g., over- or underestimation, rotation, offset), simple Taylor diagrams can be produced that include information on R^2, RMSE and Std.

3.1.1.5 Sources of uncertainty and spatial representativeness

According to 'Working Group 1 of the Joint Committee for Guides in Metrology' (2008) the ideal method for expressing uncertainty is based on three characteristics: universality, consistency and transferability. Considering this method, it is possible to evaluate the uncertainty, defined as "a parameter, associated with the results of a measurement that describes the dispersion of the values that could reasonably be attributed to the measurand".
Uncertainties related to field activities are generally related to: i) the equipment performance, ii) the methodology of measurement, iii) the sampling strategy, iv) the properties of the surface and v) the environmental conditions (Jiménez Michavila et al., 2017).
All the uncertainties associated with the measurement process are then taken into account thanks to the SI traceability, defined as "the property of the result of a measurement or the value of a standard whereby it can be related to stated references, usually national or international standards, through an unbroken chain of comparisons all having stated uncertainties" (Grkov, 2015). The unbroken chain of comparisons is called traceability chain.

fAPAR and LAI

Uncertainty sources associated with in situ PAR measurements performed using quantum sensors (e.g. SunScan, AccuPAR LP-80) are listed in Table 2. These uncertainties apply to each individual PAR measurement. Once quantified using either 'Type A' or 'Type B' evaluation, they can be propagated through the fAPAR measurement equation to derive the resulting combined standard uncertainty in the parameters.

Table 2: Uncertainty sources associated with in situ measurements of fAPAR performed using quantum sensors.

Source	Type	Description
Angular response	Systematic	Uncertainty in cosine response
Levelling	Usually random, unless mounted continually	Zenith and azimuth uncertainties
Calibration	Systematic	Uncertainty in the calibration coefficient
Radiometric resolution	Systematic	Uncertainty due to resolution of data logger to record voltage
Spectral	Mostly systematic	Uncertainty in the spectral range/response not equating to true PAR response

The uncertainties associated with in situ measurements of the fraction of intercepted PAR (FIPAR) derived using multi-angular measurements of gap fraction (e.g., LAI-2200C) are a function of several components, including angular response, instrument leveling, sampling, sky uniformity, and in the case of DHP, image classification and exposure settings (Table 3).

Table 3: Uncertainty sources associated with in situ measurements of FIPAR derived from multi-angular measurements of gap fraction.

Source	Type	Description
Angular response	Systematic	Refers to lens angular calibration
Levelling	Random	Zenith and azimuth uncertainties
Sampling	Random	Uncertainty due to spatial heterogeneity and the sampling performed (i.e. variability in gap fraction)
Image classification	Random	Uncertainty introduced by the operator during image classification in CAN-EYE
Exposure settings	Systematic and random	Uncertainty in gap fraction due to DHP under or overexposure
Sky uniformity	Random	Uncertainty due to changes in illumination conditions during measurements

Like fAPAR, the uncertainty associated with in situ LAI measurements can be evaluated as a function of several components, including uncertainties due to instrument leveling, sampling, and in the case of DHP, image classification. An additional source of uncertainty in the case of LAI is differences between analysis methods. In terms of instrument leveling, a relative standard uncertainty of approximately 2% is quoted by Origo et al. (2017) in the case of LAI, whilst the experiments conducted to assess the influence of different operators on image classification yielded relative standard uncertainties of 11% for 'effective' LAI (estimated from light extinction for a horizontally homogeneous medium) and 12% for 'true' LAI.

LCC

The uncertainty in individual in situ LCC measurements includes contributions from two main sources: i) those uncertainties inherent to the optical chlorophyll meter itself (e.g., SPAD-502), and ii) those related to the calibration function. The uncertainties inherent to the optical chlorophyll meter are easily assessed using 'Type B' evaluation, and include accuracy, repeatability, reproducibility, temperature drift, and resolution.
In addition to the uncertainties inherent to the optical chlorophyll meter, the uncertainties related to calibration function also incorporate those associated with the instruments and apparatus used to determine LCC spectrophotometrically. These include various uncertainty sources related to the spectrophotometer (i.e. photometric accuracy, repeatability, noise, drift, stray light, baseline flatness, and resolution), in addition to the volume of extraction solvent released by the dispenser, and the area of the leaf disc extracted by the cork borer. With the exception of the latter term, which must be evaluated by 'Type A' evaluation, these uncertainties can be assessed using 'Type B' evaluation.

3.1.2 Novel photosynthesis-related variables

3.1.2.1 Specific Objectives

The objective is to collect in situ measurements of the novel photosynthesis related variables to assess the quality of the corresponding FLEX products retrieved with the L2C processor. While LCARC, FQE, RED and ETR can be directly measured under field conditions on the ground, there are no methods available that allow directly measuring APAR_chl and fesc. For this reason, the two latter variables cannot be directly validated. For the validation of the other four variables (LCARC, FQE, RED and ETR) direct measurement protocols and techniques are (partly) available. However, due to the fact that FLEX will be the first satellite mission providing these variables, new sampling and upscaling approaches (leaf to canopy level) must be developed to ensure a proper validation of the satellite products. In this context, we suggest a close collaboration between the direct L2C product validation activities within FLEX DISC and the ESA project 'Fiducial Reference Measurements for Fluorescence' (FRM4FLUO) to develop adequate sampling and upscaling techniques for the validation of the novel photosynthesis related variables.

3.1.2.2 Description and justification of the methodology

LCARC

Since the destructive sampling of leaf pigments, such as chlorophyll and carotenoids, is labor, time and cost intensive, we suggest to measure LCARC non-destructively by deriving it from hyperspectral leaf reflectance measurements that can be collected with handheld devices either having an internal light source (e.g., PolyPen (Photon System Instruments, Czech Republic)) or devices that use the sunlight (Fluowat connected to a spectrometer). Based on the collected leaf reflectance data two strategies can be applied to derive information on LCARC. i) The Carotenoid Reflectance Indices CRI1 and/or CRI2 (Gitelson et al. 2002) can be applied and subsequently empirical relationships reported in literature can be used to convert the indice values to real LCARC in µg m^{-2} or ii) the newest version of the leaf radiative transfer model PROSAIL (PROSPECT-PRO, Féret et al. 2021) can be numerically inverted to determine LCARC in µg m^{-2}.

FQE, ETR and RED

FQE, ETR and RED can be measured at leaf level using active sensing techniques. The second generation of the miniaturized pulse-amplitude modulated photosynthesis yield analyzer (MiniPAM II) (Walz, Germany) and the monitoring pulse-amplitude modulated photosynthesis yield analyzer (MoniPAM) (Walz, Germany) are the most widely used instruments to measure the three novel photosynthesis related variables. However, a direct comparison of the three parameters measured on the ground with pixel values of the corresponding FLEX products is not meaningful because FLEX will provide products at canopy scale, while MiniPAM II and MoniPAM use active sensing techniques and provide information at leaf level. Because of the strong heterogeneity and leaf angle dependencies of these quantities, scaling is necessary.
Furthermore, PAM fluorometry does not provide absolute values of FQE or the RED yield that is comparable to the RED retrieved as the L2C FLEX product. PAM fluorometry measures the response to a weak, modulating measurement light, and all measurements are relative to measurements of a specific state of the photosynthetic apparatus. The measurements require anchoring to an absolute value, which can be obtained with complementary time-resolved fluorescence measurements.
Thus the following is needed:

- concurrent time-resolved fluorescence and PAM measurements to anchor the PAM derived quantities (Fo, Fs ,Fm and Fm').
- continuous PAM measurements

The scaling of PAM measurements from leaf to canopy is necessary, however, due to the large heterogeneity it is infeasible to sample a sufficient number of leaves to obtain representative measurements. Scaling is possible in the following manner:

- A radiative transfer model (e.g. SCOPE) is used to estimate the light and temperature distribution in the stand. The radiative transfer model is tuned to measured reflectance spectra for this purpose.
- An illumination and temperature response of leaf FQE is estimated from PAM measurements, leading to:

$$FQEl = f(illumination, temperature)$$

- The canopy effective FQE is calculated by first integrating FQE*APAR_chl over the leaf illumination and temperature probability density function, and then normalizing by the APAR_chl of the entire canopy:

$$FQE = \frac{\int_{leaves} FQEl \cdot APAR_{chl\ leaf} dl}{APAR_{chl}}$$

A similar approach can be followed for RED:

- First, RED is converted into an absolute value of RED yield (PhiN). The illumination and temperature response of leaf PhiN is then established
- Integration over the canopy is carried out using the light and temperature distribution in the canopy:

$$RED = \int_{leaves} \Phi_N \cdot APAR_{chl} dl$$

PAM measurements provide an absolute value of photochemical yield PhiP, and it is unnecessary to anchor these using time resolved fluorometry. Multiplication of PhiP by APAR_chl on the leaf level provides a leaf-level measurement of ETR. Scaling this to the canopy level requires a similar approach as for RED, notably:

- Establishing the relationship between PhiP and irradiance and temperature: $\Phi_P = f(irradiance, temperature)$
- Integration of PhiP*APAR_chl over the canopy:

$$ETR = \int_{leaves} \Phi_P \cdot APAR_{chl} dl$$

Alternatively to the upscaled PAM-fluorecence lifetime measurement of FQE, Yang et al. (2020) derived FQE indirectly from FloX (JB-Hypectral Devices GmbH, Germany) measurements at canopy level. This approach involves the reabsorption correction using either FCVI or radiative transfer inversion of fAPAR_chl and fesc.

To further test and develop these methods and the associated software, analysis of existing datasets such as those of AustroSIF, FLEX campaigns and new dedicated field campaigns are needed to collect canopy reflectance and SIF measurements (e.g. with FloX devices) together with active leaf measurements of FQE, ETR and RED (e.g. with MiniPAM II and MoniPAM) to develop leaf to canopy scaling functions for the three parameters. One opportunity to collect data for the development of the scaling functions

could be the ESA project FRM4FLUO. This ideally also includes the use of time-resolved fluorescence for the absolute value of FQE.

3.1.2.3 Data requirements

Below the auxiliary data required for the L2C novel photosynthesis related variables validation are listed:

i. geolocation information to account for accurate spatial comparison between in situ measurements and corresponding FLEX pixels
ii. land use/cover information to develop an appropriate spatial sampling strategy that provides information on the heterogeneity of the sampling area
iii. topographic information in the form of digital elevation models to take into account effects caused by differences in elevation and slope

3.1.2.4 Data availability

In contrast to the L2C traditional biophysical variables that are/were sampled by different networks to validate corresponding satellite products, there are no networks existing measuring the novel photosynthesis variables because FLEX will be the first satellite mission delivering those products. For this reason, field campaigns have to be conducted in the commissioning and operational phase of FLEX to directly validate the novel photosynthesis variables.

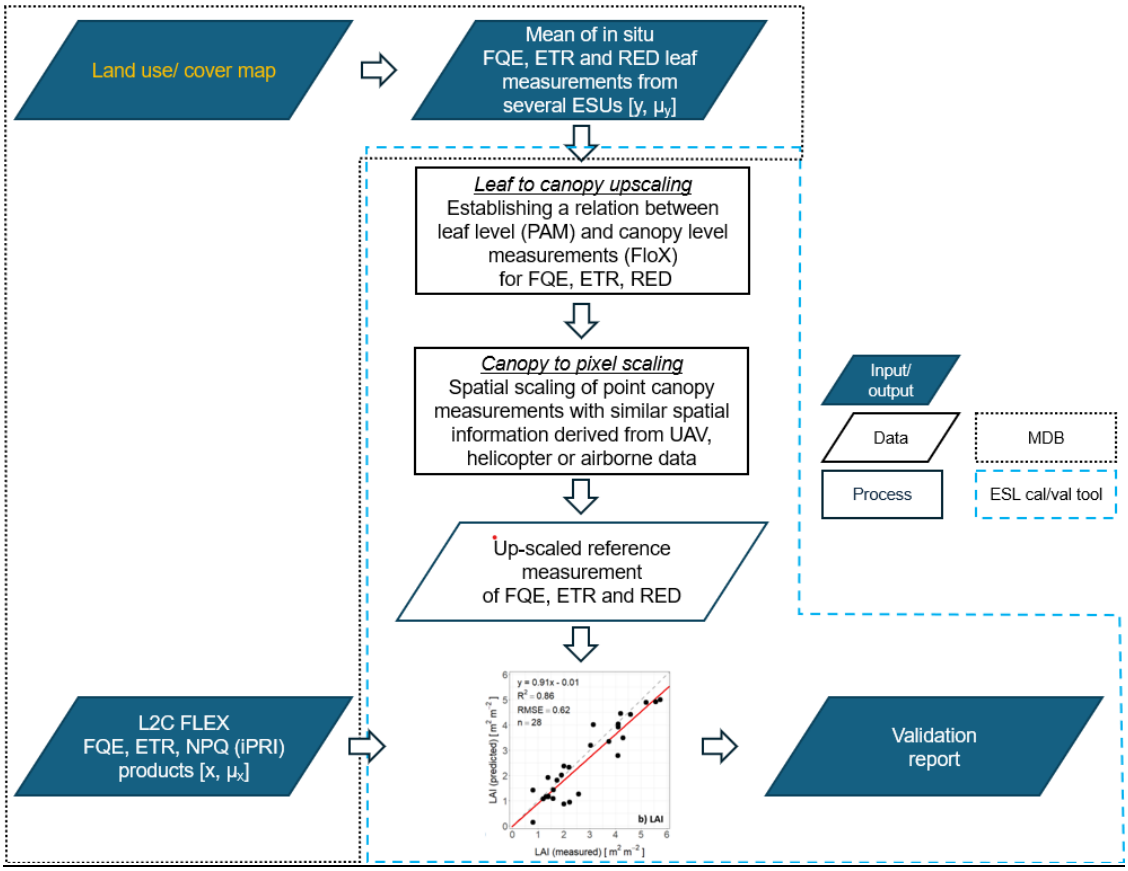
3.1.2.5 Algorithm description

While LCARC can be validated in the same way as the traditional biophysical variables (cf. solution 1 in section 3.1.1.4) using the vegetation index Pigment Specific Simple Ratio (PSSR = B08 / B02) (Blackburn 1998) for the spatial scaling, a different approache will be used for the direct validation of the remaining novel photosynthesis related variables. Following solution 3 FQE, ETR and RED measurements are collected from several ESUs to take into account the spatial variability of the variables. The number of sampled ESUs depends on the number of land cover types (heterogeneity of a FLEX pixel) and the weight of a single location measurement representing a land cover type can be determined from its percentage coverage.
An important step in the validation of the L2C products (FQE, ETR, RED) is the upscaling of the leaf level measurements to the canopy scale. Currently, the required upscaling approaches are not available but it is planned to develop them based on the data that will be collected in the project FRM4FLUO. Furthermore, we plan to use the knowledge and the data from FRM4FLUO to develop validation tools for FQE, ETR and RED that will have the following names:

- FQE - *L2 FQE Val Campaign*
- ETR - *L2 ETR Val Campaign*
- RED - *L2 RED Val Campaign*

i. Cal/Val algorithm overview and algorithm flowchart

Solution 3 - Multiple location measurements with leaf to canopy and canopy to pixel upscaling



ii. Steps involved in reading and ingesting data (description)

Validation software - Solution 6

1. Input: Reading csv file containing value(s) of the novel photosynthesis related variable in situ measurements with corresponding x and y coordinates (UTM format).
2. Quality control of the novel photosynthesis related variable in situ measurements.
3. Averaging novel photosynthesis related variable measurements and corresponding x, y and z coordinates sampled at the same position/ESU
4. Weighted averaging of all sampled measurements within one FLEX pixel according to the percentage coverage of the land cover type a sample belongs to.

5. Applying function to upscale the averaged measurement from the leaf to the canopy scale.
6. Developing a spatial transfer function developed connecting in situ FQE, ETR and RED measurements upscaled to the canopy level with the same variables measured from UAV, helicopter (both equipped with AirFloXes) or aircrafts (HyPlant, IBIS).
7. Applying the transfer function to the spatial high-resolution UAV and airborne data to generate a map of the target variable and aggregation of this map to 300 m spatial resolution.
8. Comparing in situ upscaled novel photosynthesis related variable measurements with pixel values of the corresponding FLEX L2C product using different metrics metrics (e.g., R^2, RMSE, Std, Bias).
9. Output: Generating validation report providing goodness-of-fit metrics and visualization of the validation results in the form of scatter plots.

iii. Quality checks needed on the reference and auxiliary data

Prior to upscaling, quality control should be carried out to screen the in situ measurements for poor quality data. Any measurements of the in situ data set with a value of greater than two standard deviations from the mean should be examined to assess its validity. If the measurement is determined to be spurious, it should be discarded prior to further analysis.

iv. Colocation procedures to create match-up pairs including aggregation and transfer functions used to upscale

Collocation procedures for comparing in situ reference data and FLEX products are carried out as follows:

Temporal alignment: FQE, ETR and RED are highly dynamic variables because they depend on the prevailing illumination conditions and the current plant status , i.e. the angular position of the sun and illumination intensity, and plant physiological condition (e.g. stress or no stress). For this reason, in situ reference measurements should be collected timely close to the FLEX data acquisition (±1 hour). Because they are also highly variable in space, it is not possible to collect a sufficient number of measurement points in such a short period of time. For this reason the responses of PhiN, PhiP and PhiF (FQE) to illumination and temperature are monitored over multiple diurnal cycles around the day of overpass (e.g. +/-3 days). These relationships are then used in the scaling to the stand level, at the illumination and temperature of the overpass. This alleviates the necessity for intense measurement campaigns with multiple instruments at the overpass time.

The indirect method to estimate FQE, notably via the inversion of hyperspectral measurements and SIF, is applied to measurements carried out as close as possible to the overpass time (e.g +/- 1 hour).

Spatial alignment: For the validation solution 3 it will be sufficient to measure the specific location of the in situ measurements with a standard GPS handheld device that provides an accuracy of a few meters in the x, y and z dimensions. However, in case a RTK GPS device is available, it should be used, since it provides x, y and z information with only small deviations in the range of centimeters.

v. Comparison metrics and expected output/report

Error evaluation will consist of accuracy, precision and uncertainty evaluated by several metrics reporting the goodness of fit between the FLEX novel photosynthesis related products and the corresponding in situ reference dataset. Commonly, accuracy represents systematic errors while precision represents the dispersion of product retrievals around their expected value. Metrics of accuracy and precision are often computed as the statistical mean bias, standard deviation (Std), Root Mean Square Error (RMSE), and the linear regression (R^2) of the difference between L2C from satellite products and the corresponding reference estimates. Besides standard scatter plots providing information about the goodness-of-fit of in situ and satellite data (e.g., over- or underestimation, rotation, offset), simple Taylor diagrams can be produced that include information on R^2, RMSE and Std.

3.1.2.6 Sources of uncertainty and spatial representativeness

According to 'Working Group 1 of the Joint Committee for Guides in Metrology' (2008) the ideal method for expressing uncertainty is based on three characteristics: universality, consistency and transferability. Considering this method, it is possible to evaluate the uncertainty, defined as "a parameter, associated with the results of a measurement, that describes the dispersion of the values that could reasonably be attributed to the measurand".

Uncertainties related to field activities are generally related to: i) the equipment performance, ii) the methodology of measurement, iii) the sampling strategy, iv) the properties of the surface and v) the environmental conditions (Jiménez Michavila et al., 2017).

All the uncertainties associated with the measurement process are then taken into account thanks to the SI traceability, defined as "the property of the result of a measurement or the value of a standard whereby it can be related to stated references, usually national or international standards, through an unbroken chain of comparisons all having stated uncertainties" (Grkov, 2015). The unbroken chain of comparisons is called traceability chain.

In addition, further uncertainties will be introduced through the scaling of the in situ FQE, ETR and RED measurements from the leaf to the canopy and from the canopy point measurement to the FLEX pixel. These uncertainties also include the uncertainties from the measurements that will be included in the scaling procedures (e.g., FloX,

AirFloX, HyPlant). One goal of FRM4FLUO will be the identification of the main uncertainty sources that contribute to the overall uncertainty budget of the reference measurements used to validate the FQE, ETR and RED product of FLEX. As soon as the results from FRM4FLUO are available we will update this section of the L2C validation plan.

Table 4: Uncertainty sources associated with in situ measurements of FQE, ETR and RED derived from active pulse-amplitude modulation measurements.

Source	Type	Description
Levelling	Random	Zenith and azimuth uncertainties
Sampling	Random	Uncertainty due to spatial heterogeneity and the sampling performed
Calibration	Systematic	Uncertainty in the calibration coefficient
Radiometric resolution	Systematic	Uncertainty due to resolution of data logger to record voltage
Spectral	Mostly systematic	Uncertainty in the spectral range/response not equating to true PAR response

3.2. Indirect validation

3.2.1. Traditional biophysical variables

3.2.1.1. Specific Objectives

To assess the spatio-temporal consistency, and the consistency of the mean and variability of the L2C products with available alternative satellite data products of the LAI, fAPAR and LCC variables, and that of ETR, RED, FQE and fesc with alternative products retrieved from high-resolution field and satellite data.

3.2.1.2 Description and justification of the methodology

Two ways of indirect validation will be used:

1. comparison with existing global products (see Table 3.2.1)
2. retrieval of target variables with established algorithms
    a. from other satellite data
    b. from data from ground spectrometers (see L2B Cal/Val plan [OD-02])

Direct validation is often constrained by the availability of field measurements, which can be sparse and unevenly distributed across different regions. Intercomparison allows for the assessment of the target variable over larger areas by using existing datasets (when available, such as Copernicus products, see Table 3.2.1) and model inversions that are already validated or widely accepted in the scientific community (such as PROSAIL). By leveraging cross-product comparisons and model retrievals, indirect validation provides a comprehensive consistency assessment of target variables with the L2C processor (L2PP).

Table 3.2.1 - Description of continuous EO products available for cross-comparison.

Satellite product	**Spatial resolution**	**biophysical variable**
Copernicus Global Land Monitoring service	~ 300 m	LAI, fAPAR
ESA CCI[6]	1 km300 m	LAI, fAPAR, FQE
MODIS (MODIS)[7]	500 m	LAI, fAPAR
Copernicus HR-VPP	10 m	LAI, fAPAR
Sentinel-2 biophysical processor	20 m	LAI, LCC, fAPAR
LSA SAF[8]	1000 m	LAI, fAPAR

LAI, fAPAR

LAI and fAPAR are provided by the majority of the datasets coming from polar-orbiting (Aqua/Terra, Sentinel-2, 3) and geostationary (Meteosat) satellites. Additionally, LAI and fAPAR will be retrieved from ground-measured reflectance and Sentinel-2 NRT images.

LCC

There is no continuous LCC product available at the moment. A series of static maps was developed by Xu et al., (2022, https://doi.org/10.1109/TGRS.2022.3204185) from MODIS data and by Croft et al., (2020, https://doi.org/10.1016/j.rse.2019.111479) from MERIS/OLCI data. The Sentinel-3 provides a unitless OLCI Terrestrial Chlorophyll Index (OTCI) as Level-2 product. In order to retrieve LCC with the NRT latency, Sentinel-2 biophysical processor will be used. Biophysicall processor retrieves Canopy Chlorophyll Content (CCC = LAI * LCC), which can be converted to LCC by division to LAI, retrieved with the same algorithm. Additionally, LCC will be retrieved from ground-measured leaf and canopy reflectance.

6

7 https://ladsweb.modaps.eosdis.nasa.gov/search/

8 https://lsa-saf.eumetsat.int/en/data/products/vegetation/

3.2.1.3 Data availability

Copernicus products for indirect validation, including Sentinel-2 images, are distributed under open license in NRT. Their download for the region of interest is triggered through the OpenEO framework.

ESA CCI products are openly available, but they do not overlap with the operational phase of FLEX. If the product generation is continued operationally under Copernicus, then they will be available as well. The products have to be sourced through an ftp and clipped to the regions of interest.

MODIS products are distributed through various platforms. On the AppEEARS platform the pre-processing is done on the server side, thus, this platform will be used to source MODIS products.For the intercomparison, the following requimements apply:

- The inclusion of all biomes, including agricultural areas, needleleaf and broadleaf deciduous and evergreen forest, grassland, savannahs, shrublands and tundra.
- The inclusion of homogeneous and heterogeneous landscape, to evaluate the effect of subpixel heterogeneity.
- The inclusion of flat and undulating terrain, to evaluate the effect of topography on the L2C products

Before launch, a number of synthetic scenes will be used for evaluation of the algorithm. The findings of this evaluation will support the development of the intercomparison and indirect validation strategy.

Intercomparison with global datasets can be performed at any point on the land.

Ground spectra for retrieval will be sampled over the FloX network specified in L2B document [OD-02], section 3.3.

3.2.1.4. Algorithm description

All validation algorithms share the collocation and comparison steps (Figure 3.2.1). The differences lies in the source of reference variables and the respective collocation mechanism. For global products, the value of the variable is taken directly from the nearest pixel (for pixels above 300 m) or a mean (or median) value of a group of pixels. For ground-based product, the nearest FLEX value is selected for comparison. For Sentinel-2 products derived from the biophysical processor the resampling to FLEX pixels with a simple average or median will be performed.

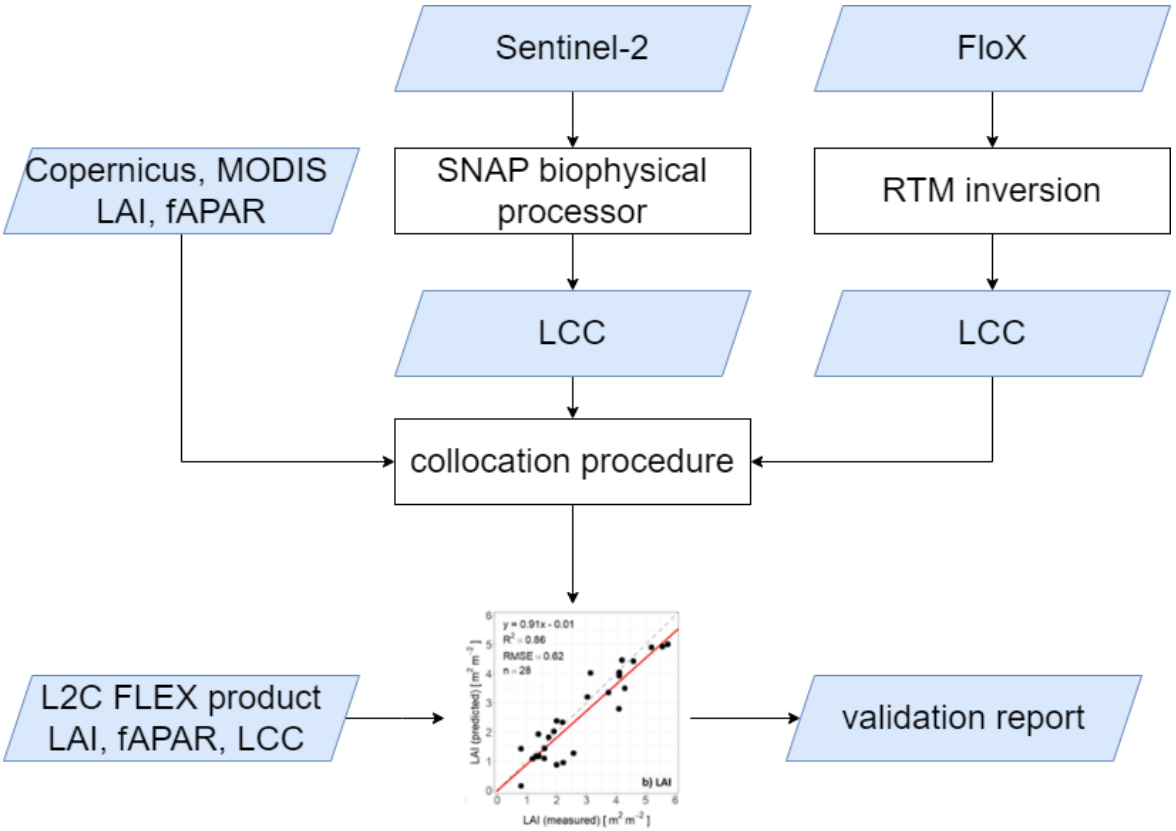


Figure 3.2.1. Indirect validation of traditional biophysical variables.

3.2.2. Novel photosynthesis-related variables

3.2.2.1. Specific Objectives

To assess the consistency and reliability of the LCARC, RED (PRI), FQE, ETR, APAR_chl and fesc variables retrieved from the FLEX campaign with the L2C processor (L2PP).

3.2.2.2 Description and justification of the methodology

Most of the novel photosynthesis-related variables require modelling for validation.

LCARC

The indirect validation of LCARC is very similar to that of LCC, as both can be achieved by inverting a radiative transfer model. However, the LCARC absorption region is narrow and thus requires hyperspectral instruments. There are two possibilities: (1) inversion from leaf spectra with PROSPEC-PRO and (2) inversion from canopy spectra with PROSAIL.

PRI (RED)

PRI computation requires two narrow bands, 531 nm and 570 nm, in the carotenoid absorption region. MODIS has long been used for PRI computations. Hyperspectral missions can be used as well. Exposed soil in the field of view influences the PRI values, as well as the sun-observation geometry and the pigment pool sizes, together overshadowing the effect of RED on PRI through the Xanthophyll cycle. To our knowledge, no satellite data products of either improved PRI or RED are available. Two interact validation attempts will be made: (1) the comparison of (not-improved) FLEX PRI to with MODIS PRI, and the comparison of improved PRI to MODIS differential Aqua-Terra (morning and afternoon overpass) PRI. This analysis can only be done if MODIS is available during the commissioning and operational phases of FLEX.

FQE, ETR, APAR_chl and fesc

FQE, ETR, APAR_chl and fesc will be validated with the forward run of the SCOPE model using high-resolution bottom of atmosphere reflectance data as input. The model will be parameterized with LAI and LCC retrieved from the ground spectra and high resolution airborne and spaceborne (e.g. PRIMSA or EnMAP) and meteorological data nearest to the FLEX overpass time. Furthermore, a product of FQE derived from TROPOSIF will be considered for evaluation of consistency of spatial patterns, seasonal cycles, mean and variability, if these are available during the operational phase of FLEX.

This is not completely independent because parts of the SCOPE model are used in the FLEX product generation chain.

3.2.2.3 Data availability

The data for indirect comparison is not available anywhere and will be computed with models. Auxiliary meteorological data for model input will be taken from ground weather stations (if available) or ERA5-Land dataset. LAI and LCC model inputs will be taken from retrievals (see section 3.2.1).

Sentinel-3 reflectance for PRI computations will be downloaded with OpenEO.

Validation of novel photosynthesis-related variables will be done at FloX network sites specified in L2B document [OD-02], section 3.3.

3.2.2.4. Algorithm description

The validation of LCARC is similar to the validation of traditional biophysicall variables. The difference is the requirement of presence of narrow bands in the carotenoind absorption region around 500 nm, which are absent in, for example, Sentinel-2.

The validation of PRI is a simple math computation on Sentinel-3 OLCI data.

The algorithm of validation of FQE, ETR, APAR_chl and fesc is presented in Figure 3.2.2. SCOPE model is parametrized with biophysical parameters retrieved from ground-measured FloX spectra and meteorological data from ERA5-Land dataset. The output variables follow the collocation procedure (selection of the nearest FLEX pixel) and comparison.

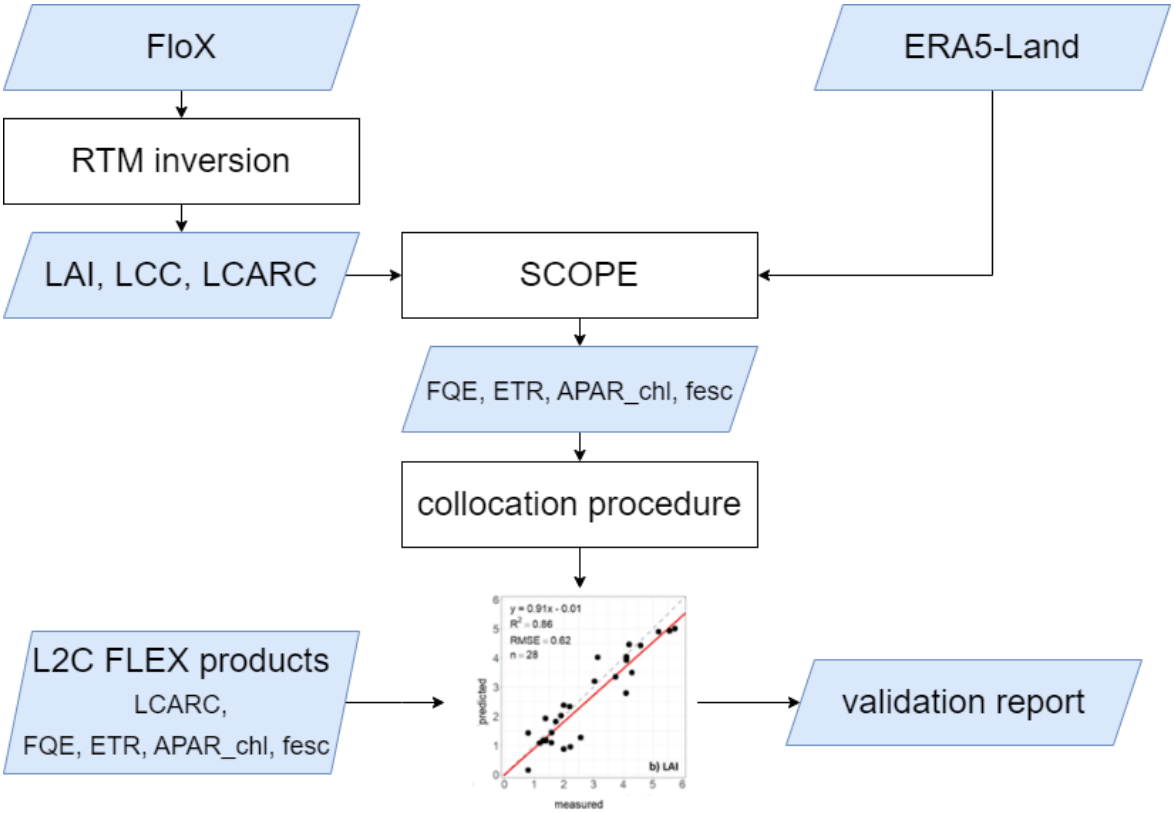


Figure 3.2.2. Indirect validation of novel photosynthesis-related variables.

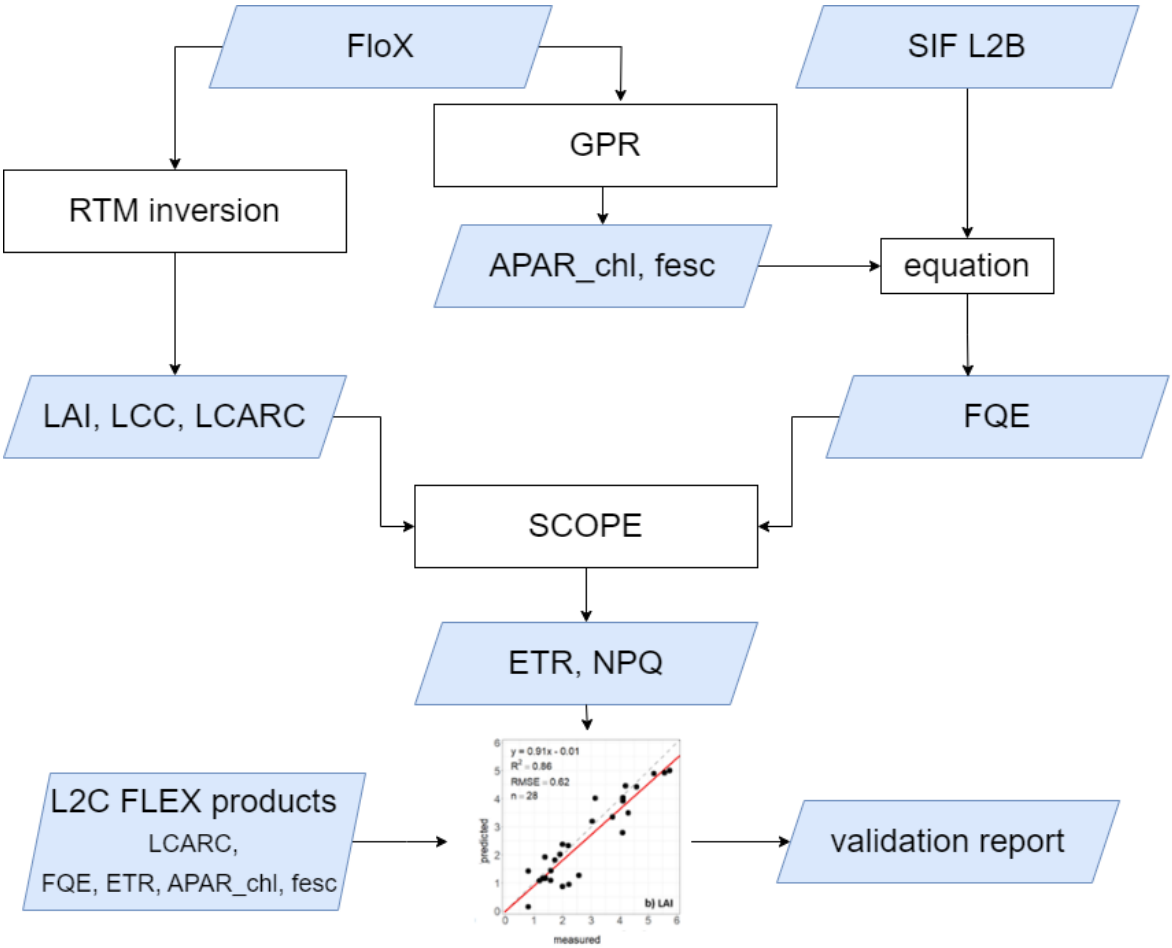


Figure 3.2.2. Indirect validation of novel photosynthesis-related variables.

4. Planning

4.1 Pre-launch activities (e.g. data acquisition, tool development, tool verification)

4.1.1 Direct Validation

Before the launch of FLEX it is planned to develop sampling and validation techniques, especially for the novel photosynthesis related products. Furthermore, the validation software (cal/val tools) for the different validation approaches will be developed within the R programming language (cf sections 3.1.1.6 and 3.1.2.6). To develop the required sampling schemes and validation approaches, and to test the validation software it will be helpful to conduct field campaigns to record in situ reference measurements of the different L2C variables with some of the proposed measurement devices listed in the sections 3.1.1.2 and 3.1.2.2. Furthermore, the in situ data collected during those campaigns could help to develop scaling functions to convert leaf measurements of FQE, ETR and RED to the canopy scale, a requirement to make leaf measurements usable for the validation of the corresponding FLEX product. The planned field campaigns within the FRM4FLUO project offer the opportunity to collect a high number of in situ data of the different L2C variables and thus we suggest to link the FLEX DISC L2C direct validation activities with the planned activities in FRM4FLUO.

4.1.2 Indirect Validation

A finite list of available global datasets will be selected for the indirect validation. The codes will be written and tested.

4.2 Commissioning phase activities (e.g. testing with commission data)

4.2.1 Direct Validation

During the commissioning phase it is planned to test the L2C algorithms and software solutions developed for the direct validation using in situ measurements collected in parallel to FLEX overflights at selected validation sites. Based on those tests problems can be identified and solved to finally produce consolidated validation approaches and software solutions for the operational phase.

4.2.2 Indirect Validation

The codes will be optimized to use with the tiled data.

4.3 Operational phase activities (testing with real data)

4.3.1 Direct Validation

During the operational phase it is planned to use the L2C algorithms and software solutions developed and consolidated in the previous phases with the final FLEX products.

4.3.2 Indirect Validation

Additional study sites may be explored based on request.

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Appendix

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