

CCI+ Vegetation Parameters

System Specification Document (SSD)

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LIST OF ACRONYMS

ATBD Algorithm Theoretical Basis Document
API Application Programming Interface
C3S Copernicus Climate Change Service

CCI Climate Change Initiative CDO Climate Data Operators

CEDA Centre for Environmental DataAnalysis
DIAS Data and Information Access Services

ESA European Space Agency

fAPAR Fraftion of Absorbed Photosynthetically Active Radiation

FTP File Transfer Protocol

IDE Integrated Development Environment

ISP Internet Service Provider

JSON JavaScript Object Notation

LAI Leaf Area Index
LAN Local Area Network

NAS Network Attached Storage
NetCDF Network Common Data Form

PUG Product User Guide

PROBA PRoject for On-Board Autonomy R&D Research and development

ROI Region Of Interest

SAN Storage Area Network

SIF Solar Induced Fluorescence

SMAC Simplified Method for Atmospheric Correction

SPOT Système Pour l'Observation de la Terre
SUSE Software- und SystemEntwicklung
TIP Two-stream Inversion Package

TOA Top of Atmosphere
TOC Top of Canopy
TDS Test Data Site

UPS Uninterruptable Power Supply URD User Requirements Document

VGT VEGETATION instrument on-board SPOT

VITO Vlaamse Instelling voor Technologisch Onderzoek

VM Virtual Machine

VP Vegetation Parameters

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1 Introduction

1.1 Scope of this document

This document describes the system developed and used for the ESA CCI Vegetation Parameters project and its elements used in cycle 2 for the generation of the LAI and fAPAR datasets (CRDP-2). The SSD exists in the context of other VP_cci documents: the User Requirements Document (URD) describes the requirements of the products to be delivered [VP-CCI_D1.1_URD] and the Algorithm Theoretical Basis Document (ATBD) describes the algorithm used for the generation of the products [VP-CCI_D2.1_ATBD].

The SSD describes the following sections:

- System overview (Chapter 2)
- System architecture (Chapter 3)
- Workflow description (Chapter 4)

1.2 Related documents

Internal documents

Reference ID	Document		
ID1	Climate Change Initiative Extension (CCI+) Phase 2 New ECVs:		
	Vegetation Parameters – EXPRO+ - Statement of Work, prepared by		
	ESA Climate Office, Reference ESA-EOP-SC-CA-2021-7, Issue 1.2, date		
	of issue 26/05/2021		
VP-CCI_D1.1_URD_V2.0	User Requirement Document: fAPAR and LAI, ESA CCI+ Vegetation		
	Parameters		
	https://climate.esa.int/media/documents/VP-CCI D1.1 URD V2.0.pdf		
VP-CCI_D2.1_ATBD_V2.2	Algorithm Theoretical Basis Document: fAPAR and LAI, ESA CCI+		
	Vegetation Parameters		
	http://climate.esa.int/media/documents/VP-CCI_D2.1_ATBD_V2.2.pdf		
VP-CCI_D4.2_PUG_V2.2	Product User Guide: LAI and fAPAR, ESA CCI+ Vegetation Parameters		
	http://climate.esa.int/media/documents/VP-CCI D4.2 PUG V2.2.pdf		
VP-CCI_D2.1_ATBD-pre-	Algorithm Theoretical Basis Document – Cycle-2 pre-processing		
processing_V1	https://climate.esa.int/media/documents/VP-CCI D2.1 ATBD pre-		
	processing v1.0.pdf		

External documents

Reference ID	Document
CCI Data	ESA Climate Office, CCI Data Standards v2.3 (CCI-PRGM-EOPS-TN-13-0009
Standards	
C3S_ATBD_SA	C3S ATBD of Surface Albedo, multi-sensor, D1.3.4-
	v2.0 ATBD CDR SA MULTI SENSOR v2.0 PRODUCTS v1.1

2 System overview

2.1 Main function and Processing chain

The main function of the VP_cci system is the repeated generation of the Vegetation Parameters products with an increasing number of input datasets (multi-sensor and multi-instrument) over the cycles and algorithms which undergo updating.

Overall, there are 4 separate steps in the processing: (1) the acquisition of the input data (level 1), (2) the pre-processing per sensor, (3) the retrieval algorithm OptiSAIL to generate LAI and fAPAR, and (4) the repackaging of the data.

In the first step, all level 1 input satellite imagery is downloaded. The data used is further described in section 4.1. The second step (see also section 0) includes the projection to a common grid and organization of the input data in 10°x10° tiles. Then these tiles are atmospherically corrected to Topof-Canopy reflectance data (TOC). The third step starts when all TOC data is available and consists of the retrieval algorithm to calculate LAI and fAPAR (see section 4.2.3). At last, the data are prepared to be uploaded to CEDA (see section 4.3).

In cycle 1, we start directly at step 3 since the input TOC reflectances are already available.

2.2 System requirements

The main requirement is the system is to generate the Vegetation Parameters products according to the algorithm defined in the ATBD [VP-CCI D2.1 ATBD] and the URD [VP-CCI D1.1 URD]. These requirements are based on the system requirements formulated in the Statement of Work of the ITT (see Table 1).

Table 1: System requirements from the ITT

ID	Requirement description	
R-19	The contractor shall ensure that the system is adequately dimensioned to accommodate the growing volumes of input and output data, and the increasing computational loads needed to process, re-process, quality control, validate, and disseminate multi-decadal, global, ECV data products, of the required climate quality, in a timely manner.	
TR-8	The Contractor shall provide the required high performance processing resources necessary and perform the processing.	
TR-28	Given the large amounts of data to be processed, the Contractor shall develop an automated high performance processing chain. This processor shall be implemented on a sufficiently powerful (possibly distributed) computing infrastructure that is capable of processing and reprocessing all the required products within the project schedule.	

In addition, the system set-up should be able to generate the products in the format as defined in the contract and described in the Product User Guide (PUG) [VP-CCI D4.2 PUG]. This means that the processing system should allow both tile-based and site-based processing.

3 System architecture

3.1 High-level system decomposition

The central component of the VP_cci system is the LAI and fAPAR retrieval process. It relies on efficient selection of input products based on observation time and coverage area. To enable this, a Data Discovery process builds a database with a catalogue of all available data for supported sensors, along with descriptions of sensors and product layouts. For some sensors, data may not be available in the processing environment, and in that case, it needs to be downloaded by a Data Acquisition process. The LAI and fAPAR retrieval process expects tiled TOC data, with uncertainties and various pixel status masks, so Pre-processing to obtain this data may be a prerequisite. Finally, the generated data is prepared by a Repackaging and Transfer process for public distribution. An illustration of these components can be found in Figure 1.

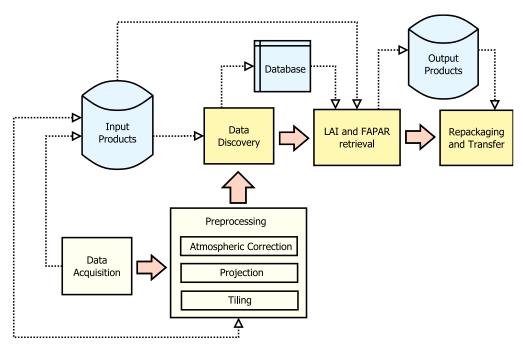


Figure 1: High-level system decomposition

Given the large amount of data that needs to be processed, there is a clear need for a distributed processing system, which is provided by the VITO's Hadoop cluster. Input data products for all sensors used in cycle 1 of this project are already available in the data archives on the NetApp storage system at the VITO processing centre. The Python programming environment is used for the development of all tooling and workflows around the LAI and FAPAR model implementations, with the PySpark library functioning as the interface to the Hadoop cluster through the Spark distributed processing engine.

3.2 Processing Environment

VITO has an energy efficient Tier 2 data centre. The computer rooms have typically an area of 8 x 8m and are filled with racks, setup in a cold aisle containment. All computer rooms have power supply redundancy using a UPS system.

3.2.1 Storage infrastructure

VITO has set-up a hybrid scale-out Storage System that unifies its SAN and NAS infrastructure, for the flexible storing and presenting of data towards the different processing chains and delivery services. The unique NetApp Storage Virtual Network technology guarantees a safe and performant presentation of the data towards all different network segments.

3.2.2 Network infrastructure

VITO has separated network segments for development, test/validation and production. All production segments are separated from each other as well. The VITO internet connectivity has an upload/download capacity of **10Gbit/sec**. VITO is connected via Belnet to GÉANT/Internet2. To serve the end user community that is not connected to the GÉANT network, VITO has an internet link to the scientific and the commercial Internet of 10 Gbit/s, both being provided by the ISP Belnet. Recently the entire internal core network switching has been upgraded to 40Gbit/sec towards the central redundant firewall and to 10Gbit/sec towards all crucial Top-Of-Rack switches in the data centre upload/download capacity of 10Gbit/sec.

3.2.3 Hadoop system cluster for scalable processing and data analytics

Hadoop as a software framework for data-intensive distributed applications, is designed to process large amounts of data by separating the data into smaller chunks and performing large numbers of small parallel operations on the data. It is applied often for processing big data and performing big data analytics. The Hadoop cluster is based on the PROBA-V Mission Exploitation Platform (MEP), a private cloud environment, with a priority scheme being implemented to avoid delays in the availability of hardware resources for operational services. The platform is based on the Hortonworks distribution and Spark¹ which is used intensively to perform large parallel processing and to allow analytics on large time series of data. The operational Hadoop environment at VITO is provided with monitoring and maintenance tools. The cluster ensures high availability through an error rollover system and provides a very scalable and powerful cluster with direct access to the data archives.



Figure 2: Spark monitoring tool

The VITO Hadoop cluster currently consists of 7000+ cores and 25+ TB of memory, and still expanding based on project demand. The cluster is located in a private cloud and hence shared with several other tasks embedded in the Terrascope platform². Every job submitted to this cluster is linked to a queue, and each queue has a priority level depending of the urgency of the processing. This can be configured based on urgency of (re-)processing actions. Currently the ESA CCI Vegetation Parameters project has a dedicated queue that is guaranteed to get a minimum of 5% of the total available cluster cores and memory, with a maximum of 100% if more resources are available during processing.

¹ https://spark.apache.org/

² https://terrascope.be/en/services



Figure 3: Cluster resource monitoring

3.2.4 Algorithm development

The VITO cloud system enables dynamic resource provisioning, and it is therefore providing a performing and scalable solution. OpenStack is used as cloud middleware for a private cloud solution at VITO. Pre-configured Virtual Machines (VM) are offered to the algorithm developers and can run on the OpenStack cluster at VITO, providing the environment needed for them to work with the data and develop/deploy applications on the platform, i.e. containing Integrated Development Environments (IDE), a rich set of tools and access to the complete data archive. Furthermore, users can customise this environment by downloading more data and tools. As such the algorithm developers have access to all input and intermediate datasets and can work in close cooperation with the workflow developers and hence enable a smooth transition between development and operations. These VM's enable the workflow developers to develop and test their new or revised workflows in a local Hadoop Spark environment with limited resources, before performing an acceptance test on the cluster.

Table 2 gives a general overview of all IT infrastructure that is in place to support the project. As more projects make use of the infrastructure, the number of resources will increase over time.

Table 2: IT infrastructure overview VITO Data center

COMPONENT	FUNCTIONALITY WITHIN PROJECT	TECHNICAL SPECIFICATIONS	
Network Infrastructure			
LAN/SAN Data Sharing, Data Exchange		LAN with 1/10 GBit/s (Gigabit Ethernet) based on TCP/IP with structured cabling infrastructure SAN FibreChannel 16/32 GBit/s	
Internet/Firewall	Data Sharing, Data Exchange	VITO head office internet connection: 10 GBit/s with a 1 GBit/s redundant line 10Gbit/s redundant Next Generation Firewall with identity awareness, anti-Bot&Anti-Virus, IPS, Anti-spam, application control and URL filtering	
Server Infrastructure			
Hadoop processing cluster Large scale parallel satellite data processing		Cluster with capacity of 7000+ cores and 25+ TB of memory, which can be dynamically allocated to project needs	
SUSE OpenStack Private Cloud Service hosting, R&D, data exchange, satellite data processing		18 compute nodes, hosting 300+ internal and external VMs on CentOS image	
VMWare cluster Service hosting, R&D, data exchange		6 hypervisor servers hosting 200+ virtual instances	
Storage Infrastructure			
Netapp storage Online storage of datasets environment		Capacity is 9.0 PB of mostly Near-Line-SAS disks	

Tape storage	Mrchive storage of datasets	Capability of handling LTO 4 to LTO8 tape technology. Current used capacity is 7.0 PB			
Cloud Computing					
CreoDIAS – WeKEO	I lata nrocessing and exchange	Multiple tenants setup and direct full VPN setup to the CreoDIAS backend			
AWS	Data processing and exchange	Multiple tenants setup and project-based VPN tunnels			
Remote Conferencing					
Teams & Zoom setups	Virtual and hybrid meetings	All of the VITO laptops and workstations have a MS Teams and Zoom environment setup for optimal virtual or hybrid meetings			
Conference rooms with hybrid Polycom setup	Virtual and hybrid meetings	Most of the VITO conference rooms are equiped with a Polycom Trio conferencephone, Clickshare technology and an optional camera for full virtual or hybrid meetings			

3.3 Database

3.3.1 Overview

The VP_cci processing system's LAI and fAPAR retrieval workflow relies heavily on selecting input products based on ROI and time range. This requires us to scan several large filesystem trees to discover products available at the processing centre and inspect their metadata (most notably start and end time). To avoid having to do this for every individual output product that has to be generated, we collect this data once before processing and store the results for later use.

In addition, the system needs to be extensible and flexible enough to accommodate multiple sensors, with new sensors added in subsequent project cycles. To handle this, we keep specific sensor configurations and product layout descriptions independent of the processing workflow implementation.

Finally, we want to keep track of the processing status and have the possibility to restart processing for selected products. Also, it should be straightforward to adjust processing parameters for selected products to test different configuration strategies.

To store all this information the VP_cci processing system uses a centralized database that contains:

- Processing configuration parameters per supported sensor
- Tile definitions per supported sensor
- Available input products per supported sensor
- Test data site definitions with selected years of interest
- Tasks for initiating processing and producing output products

To initialize the database, first a script <code>generate_database.py</code> registers sensor configurations, tiles and test data sites. Then a script <code>pl_cci_collect_products.py</code> traverses the selected input data directories, reads product metadata and registers available input products per sensor. This is implemented as a distributed Hadoop/Spark job to reduce running time. Once these two scripts are finished, this database content is considered to be read-only, and is never modified during processing.

Two additional scripts generate_tds_tasks.py and generate_transect_tasks.py are used to start the actual processing. These scripts insert new processing request tasks that will be picked up by the

processing workflow. Tile-based and site-based processing is handled by the same workflow, but with a slightly different workflow path optimized for different use cases.

The database structure diagram is shown in Figure 4. More information on the various tables can be found in sections 3.3.2 to 3.3.6.

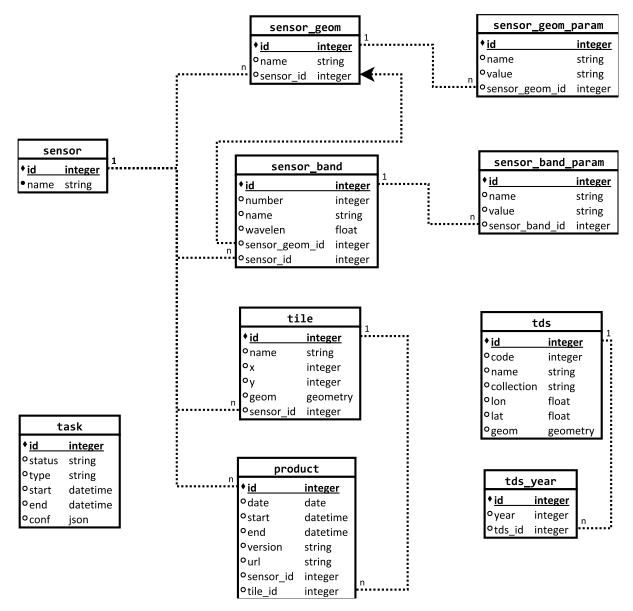


Figure 4: Database Structure

3.3.2 Sensor processing configurations

A list of supported sensors is maintained in the **sensor** table. An example of the data in this table is shown in Table 3.

Table 3: Example sensor table contents

id	name	
1	probav	
2	vgt1	
3	vgt2	

Per sensor, the **sensor_band** table stores a list of radiometric bands, each with an associated band-geometry, as illustrated in the example in Table 4.

Table 4: Example sensor_band table contents

id	number	name	wavelen	sensor_geom_id	sensor_id
1	1	band1	463.5	1	1
2	2	band2	655.0	1	1
3	3	band3	839.0	1	1
4	4	band4	1602.5	2	1

Per sensor band, the **sensor_band_param** table stores the product specific data layers to use for radiometric band, uncertainty and quality data, in addition to various related processing parameters. Table 5 shows an example of the data that is stored.

Table 5: Example sensor_band_param table contents

id	name	value	sensor_band_id
1	SDR	/LEVEL2B/RADIOMETRY/band1/TOC	1
2	SDR_uncertainty	/LEVEL2B/RADIOMETRY/band1/TOC_ERR	1
3	uncertainty_factor	= 2.236068	1
4	<pre>min_rel_uncertainty</pre>	= 0.06	1
5	quality	/LEVEL2B/QUALITY/SM_probav_v2	1
6	quality_bitmask	0x80	1
7	quality_bitvalue	0x80	1

Per sensor, there can be one or more band-geometries, depending on whether the radiometric bands are coregistered. These can be found in the **sensor_geom** table. For example, for Proba-V there are different band geometries for VNIR and SWIR bands, as shown in Table 6.

Table 6: Example sensor_geom table contents

id	name	sensor_id
1	vnir	1
2	swir	1

Per sensor band-geometry, the **sensor_geom_param** table stores the product specific data layers to use for solar and viewing angles. Snow- and cloud-mask information is also stored here as these are shared by all bands. See Table 7 for an example of the data in the database.

Table 7: Example sensor geom param table contents

id	name	value	sensor_geom_id
1	SZA	/LEVEL2B/GEOMETRY/SZA	1
2	SAA	/LEVEL2B/GEOMETRY/SAA	1
3	VZA	/LEVEL2B/GEOMETRY/VNIR/VZA	1
4	VAA	/LEVEL2B/GEOMETRY/VNIR/VAA	1
5	snow	/LEVEL2B/QUALITY/SM_probav_v2	1
6	snow_bitmask	0x4	1
7	snow_bitvalue	0x4	1
8	cloud	/LEVEL2B/QUALITY/SM_probav_v2	1
9	cloud_bitmask	0x3	1
10	<pre>cloud_bitvalue</pre>	0x0	1

3.3.3 Sensor tile definitions

Per sensor, the **tile** table contains a list of tiles, depending on the tiling grid used for the sensor's products. Note that in the processing workflow, we look for products based on their geometry, so inconsistencies between the tile numbering of different sensors are not an issue. See Table 8 for some sample database tile records.

Table 8: Example tile table contents

id	name	Х	у	geom	sensor_id
1	X00Y00	0	0	POLYGON((-180 75, -180))	1
2	X00Y01	0	1	POLYGON((-180 65, -180))	1
3	X00Y02	0	2	POLYGON((-180 55, -180))	1
4	X00Y03	0	3	POLYGON((-180 45, -180))	1

3.3.4 Sensor input products

For each available input product, its location, start time, end time, and matching tile is stored in the **products** table, as illustrated in Table 9.

Table 9: Example product table contents

id	date	start	end	version	url	sensor_id	tile_id
1	2000-01-13	2000-01-13 09:14:04	2000-01-13 09:19:53	1.0.1	file://	2	728
2	2000-01-13	2000-01-13 22:30:37	2000-01-13 22:31:16	1.0.1	file://	2	990
• • •							

3.3.5 Test data site definitions

A list of test data sites is stored in the database in the **tds** table. A test data site has a small geometry associated with it, typically covering an area of around 3 by 3 km around the test data site coordinate. An example of the records in this database table is shown in Table 10.

Table 10: Example tds table contents

id	code	Name	collection	lon	lat	geom
1	0	ABRACOS_HILL	LANDVAL V1.1	-62.3583	-10.76	POLYGON(())
2	1	ADAMOWKA	LANDVAL V1.1	59.75	51.75	POLYGON(())
3	2	AGUASCALIENTES	LANDVAL V1.1	-102.32	21.7	POLYGON(())

For each test data site there is a list of years that is of special interest, and that is stored in the tds_year table, as can be found in the sample table contents in Table 11.

Table 11: Example tds_year table contents

id	year	tds_id
1183	2006	932
1184	2007	932
1185	2008	932

3.3.6 Processing tasks

Tasks are stored in the **task** table and are the main mechanism for driving the processing workflow. They have a status that can be used to track processing progress and for reporting problems. The valid status values for a task are shown in Table 12.

Status	Meaning
PENDING	Task is waiting to be processed
RUNNING	Task is currently being processed
SUCCESS	Task finished successfully, with all timeseries dates completed
FAILURE	Task finished with an error, no timeseries dates generated
INCOMPLETE	Task finished with an error, some timeseries dates not completed
CANCELLED	Tasks is cancelled and no longer needs to be processed

Table 12: Task status values

Some example task database records can be found in Table 13.

Tab	le 13:	Exampl	e tasl	k tabi	le (contents
-----	--------	--------	--------	--------	------	----------

id	Status	type	start	End	conf
1	SUCCESS	tile	2023-09-06 10:39:32	2023-09-06 10:59:23	{}
2	SUCCESS	tile	2023-09-06 10:39:36	2023-09-06 11:45:17	{}

Tasks have a **type** parameter that indicates whether to generate a tile or a test data site product. In addition, each task has a set of configuration parameters stored in JSON format, depending on the task type. Typically, the **geom**, **start**, **end** and **interval** parameters are provided to specify the ROI and timeseries dates to be generated. Optionally a specific list of **sensors** can be requested. For an example configuration see Figure 5.

```
conf = {
  "name":
              "X19Y00"
  "geom":
              "POLYGON((10 75, 10 65.008929, ...))",
  "type":
              "tile",
  "start":
              "2019-10-01",
              "2020-12-31"
  "end":
  "interval":
              "5D"
              "10D"
  "window":
  "sensors":
              ["probav", "vgt1", "vgt2", "s3a", ...],
              "crdp2/tiles"
  "basedir":
```

Figure 5: Task configuration in JSON format

4 Workflows

The LAI and FAPAR retrieval workflow is the main component of the VP_cci processing system. It generates an LAI and FAPAR image timeseries for a specified geographical area and date range.

The timeseries date range is sampled at a specified interval, every 5 days by default. At each sample date in the timeseries, a selection is made of the available input products that overlap the area of interest and a configurable observation window around the sample date (10 days by default). The selected input data products, that may originate from a mix of different sensors, are then combined by the *OptiSAIL* model to generate an LAI and FAPAR output product, with a number of additional output layers.

The LAI and FAPAR retrieval workflow expects input products with cloud, snow and quality masks, in addition to TOC reflectance and uncertainty layers. If the required product layers are not available at the processing centre, data may need to be downloaded and/or preprocessed by applying atmospheric correction, reprojection and tiling.

A high-level view of the dataflow through the VP_cci processing system is shown in Figure 6.

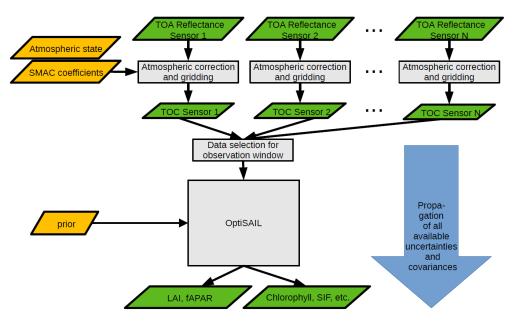


Figure 6: High-level view of dataflow

The implementation of the different workflow components is done in the Python programming language, using the PySpark API for distributed processing on VITO's Spark/Hadoop cluster environment. The LAI and FAPAR retrieval models are implemented as independent command line programs and are invoked from the workflow code through a Python wrapper layer.

4.1 Input data acquisition

The input data used in cycle 1 are intermediate data from the C3S_312b_Lot5 contract [C3S_ATBD_SA]. This dataset consists of surface reflectance data from SPOT4/5-VGT1/2 and Proba-V at 1 km spatial resolution. This dataset was already available at the processing centre. For more details see the ATBD [VP-CCI_D2.1_ATBD]. No additional data was acquired for the processing.

For cycle 2, more sensors were added to the processing, i.e. MetopA,C-AVHRR and SNPP-VIIRS. The L1B input data from these sensors were first pre-processed in the same way as was done for VGT and Proba-V in order to maximize consistency between the input data in OptiSAIL. The details of the datasets and algorithms can be found in [VP-CCI_ATBD-pre-processing].

4.2 Data processing

4.2.1 Diagram Symbols

A list of symbols used in the workflows diagrams of the next sections can be found in Table 14.

Table 14: Workflow diagram symbols

0	Workflow start
	Workflow end
\otimes	Summing junction
\Diamond	Condition
Operation	Operation
 	Parallel execution
database	Database operation
OptiSAIL	OptiSAIL process
Merge	Merge chunks process
Tilling/Proj	Tiling and projection process
Smaccl	Smaccl process
Adapt	Adapt Smaccl output process

4.2.2 Pre-processing workflow

As mentioned in section 4.1, the data used in cycle 1 were already pre-processed and available for further processing. For CRDP-2, Metop-AVHRR and VIIRS data were added as input data. These

datasets needed to be downloaded and pre-processed in the same way as the existing datasets. The pre-processing includes (i) the conversion of the input segment data needs to a regular latitude/longitude grid and split the segments into tiles, and (ii)the atmospheric correction step in which the *Smaccl* atmospheric correction model is applied to the data to obtain TOA reflectances and uncertainties. The general workflow and algorithms are explained in the ATBD of the pre-processing [VP-CCI ATBD pre-processing].

The workflow starts by scanning the filesystem for products to be pre-processed, all these products will be queued for parallel processing.

For Metop-AVHRR products, the first step is to run the the *Smaccl* atmospheric correction, this module interprets the sensor-specific encoded input segment data and generates TOA reflectances and uncertainties. This data is then read by the *Tiling and Projection* module to generate tiles on the latitude/longitude grid, in a file format that is usable directly by the LAI and FAPAR retrieval workflow.

For VIIRS products, which are provided as standard NetCDF products, the workflow is slightly different. As the first step, the *Tiling and Projection* module splits the input segment data into tiles on the latitude/longitude grid. Then, for each generated tile, the *Smaccl* atmospheric correction is run to generate TOA reflectances and uncertainties. The *Smaccl* output data then needs to be adapted for further processing by the LAI and FAPAR retrieval workflow, which is handled by the *Adapt* module.

A diagram of the Pre-processing workflow is shown in Figure 7:

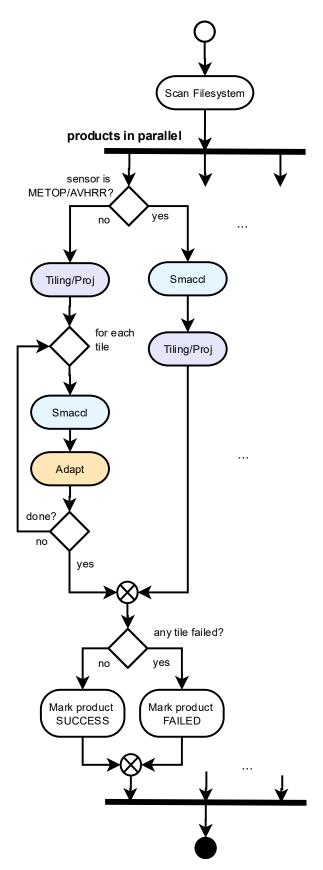


Figure 7: Pre-processing workflow

4.2.3 LAI and FAPAR retrieval workflow

4.2.3.1 Workflow driver

The workflow driver is responsible for querying the database for tasks to be processed. Each task has a set of configuration parameters, notably:

- The region of interest, this can be a larger tile or a smaller test data site geometry
- The time-series dates to be generated
- The type of task, generate a tile or a test data site product

Depending on the type of task, the workflow driver then delegates the actual processing to a sub-workflow. The workflow driver actions and decision tree are illustrated in Figure 8. A sub-workflow is scheduled to be run by a pool of worker processes, and there are different pools for tiles and sites. This enables us to run multiple sites and tiles in parallel and allows us to scale the available cluster resources according to the workload per type of task.

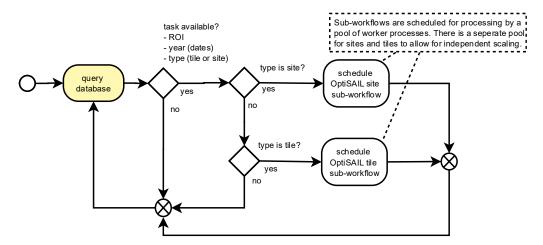


Figure 8: Workflow driver

The processing result is identical for the same location when processing it in a tile or as a site.

4.2.3.2 OptiSAIL Site Sub-Workflow

This sub-workflow uses *OptiSAIL* for LAI and FAPAR retrieval but is specifically intended to handle the small ROIs associated with the test data sites. Each *OptiSAIL* run handles only a tiny amount of data per site and takes only a very small time to complete, so this workflow does not employ any parallel processing and per site simply generates each timeseries date in sequence. This minimize the overhead associated with running tasks on the Spark cluster. As described in 4.2.3.1, a configurable number of sites can be processed in parallel using a pool of worker processes.

The input for this sub-workflow is a database task table entry, which specifies the region of interest and the time-series dates to be generated, amongst other configuration parameters. Timeseries dates are typically generated with a 5-day interval.

Next, for each time-series date, the database is queried for a list of input data products that have an observation time within a window around that date (normally 10 days) and that overlaps the area of interest. For each type of input product, the sensor configuration parameters are fetched from the database. This information is then used to as input for *OptiSAIL* (see section 4.2.4.2) to generate the LAI and FAPAR timeseries output. It is important that all time-series dates are handled sequentially in order, because *OptiSAIL* uses information acquired for the previous date.

Finally, the task status is updated in the database. If a complete time series could be generated without errors, the task is considered to be completed successfully. If the workflow was unable to generate a timeseries the task is considered to have failed. However, if a time series could be generated, despite some dates failing, the product is marked as incomplete.

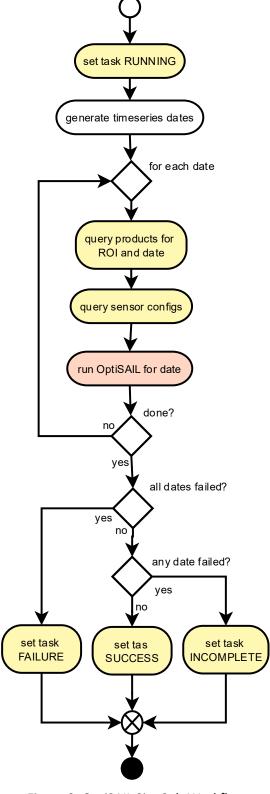


Figure 9: OptiSAIL Site Sub-Workflow

4.2.3.3 OptiSAIL Tile Sub-Workflow

This sub-workflow uses *OptiSAIL* for LAI and FAPAR retrieval and is optimized for larger ROIs. It is important that all timeseries dates are handled sequentially in order, because *OptiSAIL* uses information acquired for the previous date. To take advantage of the parallel processing infrastructure offered by the Spark cluster, this workflow splits the ROI into multiple chunks, processes the chunks in parallel, and merges the results afterwards. The input data is not actually split into chunks, only the ROI for which *OptiSAIL* generates a product is split into regions. As described in 4.2.3.1, a configurable number of tiles can be processed in parallel using a pool of worker processes.

As with the other sub-workflow, the input here is a database task table entry, which specifies the region of interest and the timeseries dates to be generated, amongst other configuration parameters. Time-series dates are typically generated with a 5-day interval.

Next, for each time-series date, the database is queried for a list of input data products that have an observation time within a window around that date (normally 10 days) and that overlaps the area of interest. For each type of input product, the sensor configuration parameters are fetched from the database. Note that for these queries, each date can be processed independently in parallel. This information is used to generate the configuration files for *OptiSAIL* (see section 4.2.4.7).

Then, as illustrated in Figure 10, the ROI is split into chunks, and all chunks are then processed in parallel. Per chunk, the *OptiSAIL* program is run sequentially for all time-series dates. This then produces LAI and FAPAR output files per chunk for all dates in the timeseries.

Next, the output files per chunks are merged into the final LAI and FAPAR product per timeseries date. In this step again all dates can be processed in parallel.

Finally, as with the other sub workflow, the task status is updated in the database. If a complete time series could be generated without errors, the task is considered to be completed successfully. If the workflow was unable to generate a timeseries the task is considered to have failed. However, if a time series could be generated, despite some dates failing, the product is marked as incomplete.

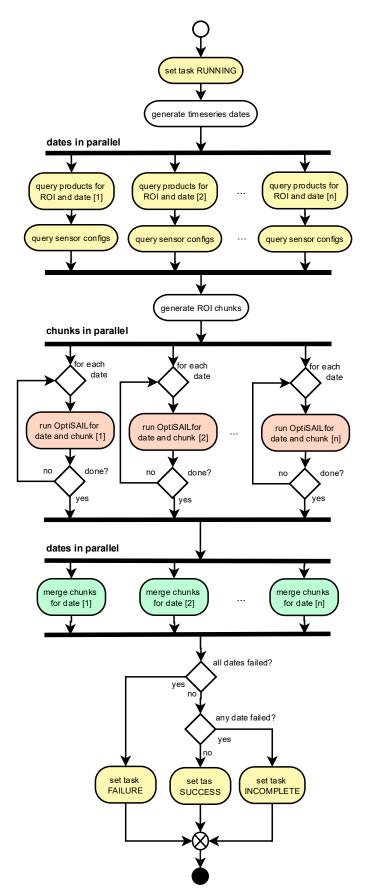


Figure 10: OptiSAIL Tile Sub-Workflow

4.2.4 Executables

4.2.4.1 Wrapper Interfaces

The *OptiSAIL* and Merge workflow operations are implemented as external command line executables. To make them callable from the workflow's Python code they are wrapped as importable Python modules. In addition, each wrapper module is implemented in such a way that it can be executed directly as a command line program, for testing purposes.

A wrapper module prepares the executable environment by configuring the dynamically linked library path, setting environment variables that affect executable initialization and optionally generating configuration files. It then runs the executable as a subprocess, while capturing output messages and runtime metrics and redirecting these to a log file.

4.2.4.2 Tiling and Projection

Takes a Level-1B segment product and transforms the raster data to a regular latitude/longitude grid (plate carrée projection) with ellipsoid WGS 1984. The data is split into tiles according to the specified tiling grid. Both Metop-AVHRR and VIIRS sensor products are supported. Output data is written in a form that is usable by the *Smaccl* and *OptiSAIL* executables described in the following sections.

Input:

- L1B segment product data, as NetCDF files
- Tile geometry definitions, as a GeoJSON file
- Target resolution, set to 1KM

Output:

- A list of NetCDF files, one per tile

4.2.4.3 Smaccl

Applies the atmospheric correction model as described in the ATBD [VP-CCI_D2.1_ATBD_V2.].

Input:

- Input product, as a NetCDF file
- Meteo data (MERRA aerosol and pressure)
- Digital elevation model (GTOPO30)
- Sensor specification and band selection
- Smac coefficients

Output:

NetCDF file

The inputs are provided through a configuration file, see section 4.2.4.7 for more information.

4.2.4.4 Adapt

This program re-inserts some NetCDF metadata that was lost by the *Smaccl* atmospheric correction process, but that is required to obtain a CF-compliant NetCDF file that can be used as input for *OptiSAIL*. More information can be found in section 4.2.2.

Input:

A Smaccl output product, as a NetCDF file.

Output:

- A CF-compliant NetCDF file, usable by OptiSAIL

4.2.4.5 OptiSAIL

This program implements the LAI and fAPAR retrieval model.

Input:

- ROI
- Date and observation window
- Input products for one or more sensors, as NetCDF files
- Input product layout specifications, including
 - Solar and viewing angles
 - TOC reflectance bands
 - Uncertainty bands
 - Cloud, snow and quality masks
- Land/Sea mask

Output:

NetCDF file

The inputs are provided through a configuration file, see section 4.2.4.8 for more information.

4.2.4.6 Merge

This program merges the chunked OptiSAIL products together as described in 4.2.3.3.

Input:

- A list of OptiSAIL output products, as NetCDF files.

Output:

A NetCDF file

4.2.4.7 Example Smaccl Configuration File

Figure 11 shows an example configuration file used by Smaccl.

```
[Paths]
         ../AVHR_xxx_1B_M03_20190703141602Z_20190703141902Z_N_0_20190703152222Z
output dir = .../AVHR xxx 1B M03 20190703141602Z 20190703141902Z N 0 20190703152222Z
output = .../AVHR_xxx_1B_M03_20190703141602Z_20190703141902Z_N_0_20190703152222Z.nc.part
merraaero = .../MERRA2_300.tavg1_2d_aer_Nx.20190701.SUB.nc4
merraptwo = .../MERRA2_300.tavg1_2d_slv_Nx.20190701.SUB.nc4
smaccoef_dir = .../COEFFS/
smaccoef_version = 3.0
dem = .../GTOPO30_DZ_MLUT.nc
faer = .../Aerosol_model_fraction.txt
[Sensor]
platform = METOP 1
sensor = AVHRR
bands = 1 2 3a 3b
[Coefficients]
k_uh2o = 1e-1
k_uo3 = 1e-3
k p0 = 1e-2
Etoa = 0
ERtoa = 0.01
Etaup = 0.05
```

```
ERtaup = 0.15
Euo3 = 0.0
ERuo3 = 0.06
Euh2o = 0.0
ERuh2o = 0.2
Epre = 1.0
ERpre = 0.0
taot = 0.5

[Sizes]
imsize = -1
nbchunk = 10

[Output]
Jacobien = False
```

Figure 11: Smaccl configuration file

4.2.4.8 Example OptiSAIL Configuration File

Figure 12 shows an example configuration file used by OptiSAIL, with some repetitive sections truncated for brevity.

```
processing_mode = tile
obs_interval_h = 240
valid_date = 20140426T12:00
n_{geometries} = 106
n_geometry_settings = 4
n_bands = 8
n_band_settings = 8
n_{obs} = 212
n_sensors = 2
n_files = 53
roi_latsouth = 45.008929
roi_latnorth = 55
roi_lonwest = 0
roi_loneast = 9.991071
slab\_size = 224
land_mask_file_id = 54
land_mask = data
land_bitmask = 0x7f
land_bitvalue = 0x01
output_retrieval = .../X18Y02_optisail_2014-04-26.nc
output_covariance = .../X18Y02_optisail_2014-04-26.nc
previous_retrieval = .../X18Y02_optisail_2014-04-21.nc
<centre_wavelengths>
1 463.5
. . .
8 1635.0
</re>
<sensor_names>
1 Proba-V_CENTER
2 VGT2
</sensor_names>
<files>
```

```
1 fqfilename .../c3s_L2B_20140421_X18Y02_114528_1KM_2_PROBAV_SM_V1.0.1.nc
. . .
53 fqfilename .../c3s_L2B_20140501_X18Y02_094348_1KM_3_PROBAV_SM_V1.0.1.nc
54 fqfilename .../land_sea_mask_1km_X18Y02.nc
</files>
<band_settings>
1 sensor_id 1
1 wavelength_ix 1
1 SDR /LEVEL2B/RADIOMETRY/band1/TOC
1 SDR_uncertainty /LEVEL2B/RADIOMETRY/band1/TOC_ERR
1 uncertainty_factor = 2.236068
1 min_rel_uncertainty = 0.06
1 quality /LEVEL2B/QUALITY/SM_probav_v2
1 quality_bitmask 0x80
1 quality_bitvalue 0x80
. . .
8 sensor_id 2
8 wavelength_ix 8
8 SDR /LEVEL2B/RADIOMETRY/band4/TOC
8 SDR_uncertainty /LEVEL2B/RADIOMETRY/band4/TOC_ERR
8 uncertainty_factor = 2.236068
8 min_rel_uncertainty = 0.06
8 quality /LEVEL2B/QUALITY/SM
8 quality_bitmask 0x00
8 quality_bitvalue 0x00
</band_settings>
<geometry_settings>
1 SZA /LEVEL2B/GEOMETRY/SZA
1 SAA /LEVEL2B/GEOMETRY/SAA
1 VZA /LEVEL2B/GEOMETRY/VNIR/VZA
1 VAA /LEVEL2B/GEOMETRY/VNIR/VAA
1 snow /LEVEL2B/QUALITY/SM_probav_v2
1 snow_bitmask 0x4
1 snow_bitvalue 0x4
1 cloud /LEVEL2B/QUALITY/SM_probav_v2
1 cloud_bitmask 0x3
1 cloud_bitvalue 0x0
</geometry_settings>
<geometries>
1 file_id 1
1 status_file_id 1
1 geometry_settings_id 1
106 status_file_id 53
106 geometry_settings_id 2
</geometries>
<observations>
```

```
1 file_id 1
1 geometry_id 1
1 band_settings_id 1
...
212 file_id 53
212 geometry_id 106
212 band_settings_id 4
</observations>
```

Figure 12: OptiSAIL configuration file

4.3 Data repackaging and transfer

Before public distribution we repackage the NetCDF output products generated by the LAI and FAPAR retrieval workflow. We implemented this in Python as a Spark/Hadoop process to reduce running time.

The repackaging process ensures that our products are compliant with *ESA/CCI Data Standards*³, which implies compliance to *CF-1.8 conventions*⁴. At this point we also include the Digital Object Identifier (DOI) assigned to us by CEDA as a NetCDF attribute.

For sites the final filename format is:

```
ESACCI-VEGETATION-L3S-VP_PRODUCTS-MERGED-site_<site-id>_<site-name>-<YYYY>-fv1.0.nc
```

And for tiles the final filename format is:

```
ESACCI-VEGETATION-L3S-VP_PRODUCTS-MERGED-tile_<tile>-<YYYYYMMDD>-fv1.0.nc
```

Repackaging also reduces the total data volume, because we remove project-internal data layers and files. We additionally merge the tiny per-date NetCDF files for test data sites into one-year timeseries NetCDF files, which greatly reduces storage overhead and number of files.

After repackaging, we obtain a filesystem hierarchy as shown in Figure 13.

```
|- sites/
|- 2000/
|- 2001/
|- ...
|- 2020/
|- ESACCI-VEGETATION-L3S-VP_PRODUCTS-MERGED-site_00001_ABRACOS_HILL-2020-fv1.0.nc
|- ESACCI-VEGETATION-L3S-VP_PRODUCTS-MERGED-site_00002_ADAMOWKA-2020-fv1.0.nc
|- ...
|- ESACCI-VEGETATION-L3S-VP_PRODUCTS-MERGED-site_00932_BILANTAO_NE_SW-2020-fv1.0.nc
|- transect/
|- 2000/
|- 2001/
|- ...
|- 2020/
|- X19Y00
|- X19Y00
|- X19Y01
|- ...
|- X20Y10
|- ESACCI-VEGETATION-L3S-VP_PRODUCTS-MERGED-tile_X20Y10-20200101-fv1.0.nc
```

³ https://climate.esa.int/en/explore/esa-cci-data-standards

⁴ http://cfconventions.org/

Figure 13: Filesystem Hierarchy after repackaging

After repackaging we transfer all data from the processing centre at VITO to the CEDA Archive⁵ using the open-source NCFTP⁶ FTP client, with the following command:

ncftpput -R -v -u <user> -p <password> arrivals.ceda.ac.uk /CCI-Vegetation-Parameters <src-dir>

⁵ https://archive.ceda.ac.uk/

⁶ https://www.ncftp.com/ncftp