TERRASCOPE SENTINEL-2

ALGORITHM THEORETICAL BASE DOCUMENT (ATBD)

S2 – TOC – V102

Reference: *Terrascope Sentinel-2 Algorithm theoretical base document S2 – TOC – V102*

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LIST OF ACRONYMS

ACRONYM	EXPLANATION
ACIX	Atmospheric Correction Inter-comparison Exercise
AOT	Aerosol Optical Thickness
ATBD	Algorithm Theoretical Base Document
ATLAS	Atmospheric Laboratory for Applications and Science
BENELUX	Belgium – the Netherlands – Luxembourg
CAMS	Copernicus Atmospheric Monitoring Service
CCI	Climate Change Initiative
CWV	Column Water Vapour
DEM	Digital Elevation Model
DISORT	DIScrete Ordinate Radiative Transfer
ECMWF	European Centre for Medium-Range Weather Forecasts
ESA	European Space Agency
EURECA	European Retrieval CArrier
fAPAR	Fraction of Absorbed Photosynthetically Active Radiation
fCOVER	Fraction of green vegetation Cover
GeoTIFF	Geostationary Earth Orbit Tagged Image File Format
GLOBE	Global Land One-km Base Elevation Project
iCOR	Image Correction for atmospheric effects
L1C	L1C
LAI	Leaf Area Index
LUT	Look-Up-Table
MEP	Mission Exploitation Platform
MODTRAN5	MODerate resolution atmospheric TRANsmission
MSI	Multispectral Instrument
NDVI	Normal Difference Vegetation Index
NRT	Near Real Time
OGC	Open Geospatial Consortium
PDP	Product Distribution Portal
PROBA-V	Project for On-Board Autonomy – Vegetation
RAA	Relative Azimuth Angle
RD	Related Document
S2	Sentinel-2
SAA	Sun Azimuth Angle
SAR	Synthetic Aperture
Sen2Cor	Sentinel-2 Correction
SOLSPEC	SOLar SPECtrum
SPOT	Satellite Pour l'Observation de la Terre
SRF	Spectral Response Function
STEP	Science Toolbox Exploitation Platform
SWIR	Short wave infrared

SZA	Solar Zenith Angle
TOA	Top-Of-Atmosphere
TOC	Top-Of-Canopy
UTM	Universal Transverse Mercator
VAA	View Azimuth Angle
VITO	Vlaams Instituut voor Technologisch Onderzoek
VNIR	Visible and Near InfraRed
VZA	View Zenith Angle
WGS84	World Geodetic System 1984
XML	Extensible Markup Language

1. Introduction

1.1. Terrascope explained

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

The offering includes
- The SPOT-VEGETATION archive
- The PROBA-V archive and current data
- The Sentinel-1 SAR data above Belgium
- The Sentinel-2 optical data above the BENELUX, soon to be expanded to Europe and Africa
- The Sentinel-3 optical and thermal Synergy (SYN) – Vegetation (VGT) data

A standard set op biophysical indicators (NDVI, FAPAR, FCOVER, LAI) derived from Sentinel-2 data is offered alongside the data.

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

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

1.2. Scope of Document

This ATBD (Algorithm Theoretical Base Document) describes the Sentinel-2 (S2) Level1C (L1C) Top-Of-Atmosphere (TOA) to Level2 Top-Of-Canopy (TOC) processing steps, embedded in the Terrascope Sentinel-2 v102 processing chain.

The document is organised as following:
- Section 2 provides an overview of all input data needed to feed the processing chain, including a description of the S2 L1C input data and ancillary data.
- Section 3 explains the output layers of the chain, available for the users.
- Section 4 provides a detailed description of the different algorithms that compose the L1C to L2 processing chain.
- Section 5 discusses the limitations of the implemented algorithms.

- Section 6 justifies the overall workflow with a quality assessment.

1.3. Description

The S2 TOC product is a geometrically and atmospherically corrected version of the original European Space Agency (ESA) L1C data with additional information on pixel classification and Aerosol Optical Thickness (AOT).

The workflow starts from L1C data of Sentinel-2 as provided by ESA (Gatti et al., 2018) [RD1], which is Top Of Atmosphere (TOA) reflectance in cartographic geometry (i.e. combined UTM projection and WGS84 ellipsoid). In the first step of Terrascope, the data are visually inspected for geometric accuracy. When the spatial shift is larger than five meter, a geometric adjustment is performed. In the next step, Sen2Cor (Mueller-Wilm et al., 2018) [RD2] classifies pixels into pre-defined categories: vegetation, bare soil, water, snow, cloud, cloud shadow, dark area, saturation or defect. The final step corrects for atmospheric effects using iCOR (De Keukelaere et al., 2018) [RD3], an image based atmospheric correction algorithm. The output of this workflow encompasses TOC reflectance for each spectral band, a scene classification layer and an AOT output layer.

The document is applicable for the Terrascope S2 v102 processing chain. The changes between v101 and v102 are listed in Table 1.1. Validation results between both versions are included in Section 6.1.

Table 1.1: List of changes between TERRACOPE Sentinel-2 v101 and v102

Adaptations between v101 and V102	Clarification
Scene classification	
Update of Sen2Cor version (v2.3 → v2.5.5)	On 23/03/2018 a new version of Sen2Cor was released (v2.5.5). [RD2]
Atmospheric correction	
Update Spectral Response Function (SRF)	On 19/11/2017 ESA launched an update of the SRF (v3.0) (ESA, 2017).
AOT fall back solution	To handle inaccurate image-based AOT retrieval due to high cloud cover or failure.
Bilinear interpolation of AOT values	The AOT result of iCOR is a grid at 60 m resolution. These values have to be resampled to 10 and 20 m. In the previous version a nearest neighbour interpolation was implemented. This is changed into a bilinear interpolation technique.

Adaptations between v101 and V102	Clarification
Output products	
AOT layer at 60m	An additional layer is made available to the users.
Saturation of TOC reflectance at a value of 200% instead of 100%	To avoid saturation in high reflective objects (e.g. clouds) a higher saturation level was defined

1.4. Feature added value/use case

The atmospheric impact on the TOA reflectance differs for each spectral band. In data assessment studies (e.g. band ratios, time series analysis or quantitative studies), atmospheric disturbances and inaccurate geolocation will hamper a good analysis. The Terrascope platform provides a solution for users wanting to work with atmospherically and geometrically corrected S2 data by making TOC products available. All S2 data covering Belgium, the Netherlands and Luxembourg from the start of the mission (23/06/2015 for S2A and 7/03/2017 for S2B) are available on the platform. The TOC products are accompanied with pixel classification layers to ease interpretation of results.

1.5. Related documents

Table 1.1 lists the related documents (RD) that are complementary to this ATBD. Other Reference Documents (ORD) are listed in Section 7.

Table 1.2: List of related documents

[RD1]	Gatti, A., Galoppo, A. Castellani, C., Carriero, F. Sentinel-2 Products Specification Document, REF: S2-PDGS-TAS-DI-PSD issue 14.5,20/03/2018 https://sentinel.esa.int/documents/247904/685211/Sentinel-2-Products-Specification-Document
[RD2]	Mueller-Wilm, U., Devignot, O., Pessiot, L. (2018) S2 MPC Sen2Cor Configuration and User Manual. Ref. S2-PDGS-MPC-L2A-SUM-V2.5.5. http://step.esa.int/thirdparties/sen2cor/2.5.5/docs/S2-PDGS-MPC-L2A-SUM-V2.5.5_V2.pdf
[RD3]	De Keukelaere, L., Sterckx, S., Adriaensen, S., Knaeps, E., Reusen, I., Giardino, C., Bresciani, M., Hunter,P., Neil, C., Van der Zande, D. & Vaiciute, D. (2018). Atmospheric correction of Landsat-8/OLI and Sentinel-2/MSI data using iCOR algorithm: validation for coastal and inland waters. European Journal of Remote Sensing., Vol 51, 525-542. https://doi.org/10.1080/22797254.2018.1457937
[RD4]	Paepen, M., et al. (2019) Terrascope Sentinel-2 Product User Manual V1.1

2. Input

2.1. General

We start from the S2 L1C data products that can be freely downloaded from the Copernicus Open Access Hub (https://scihub.copernicus.eu/dhus/#/home). The data are distributed in granules, also called tiles, which are 100x100 km² ortho-images in Universal Transverse Mercator World Geodetic System 1984 (UTM/WGS84) projection with an overlap of 9.8 km between overlapping tiles. The tiling grid can be downloaded from Sentinel-2 tiling grid.kml. The L1C data are TOA reflectance projected in UTM zones of the WGS84 ellipsoid.

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

- 4 bands at 10m spatial resolution: blue (490nm), green (560nm), red (665nm) and near infrared (842nm).
- 6 bands at 20m spatial resolution: 4 narrow bands for vegetation characterization (705nm, 740nm, 783nm and 865nm) and 2 larger SWIR bands (1610nm and 2190nm) for applications such as snow/ice/cloud detection or vegetation moisture stress assessment.
- 3 bands at 60m spatial resolution, mainly for cloud screening and atmospheric corrections (443nm for aerosols, 945 for water vapor and 1375nm for cirrus detection).

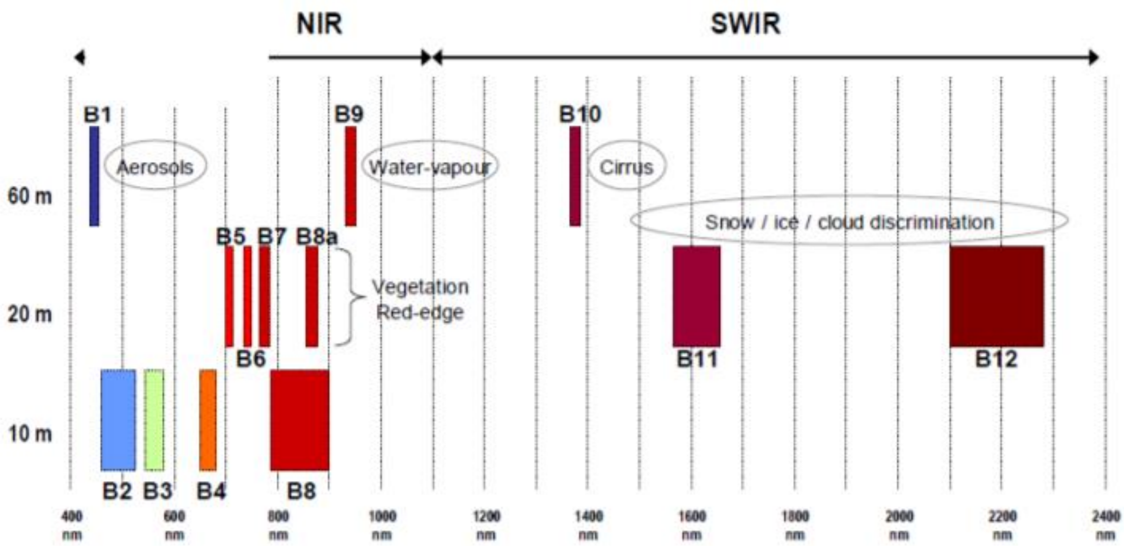


Figure 2.1: S2-MSI Spectral-Bands versus Spatial Resolution Reference [RD3]

More info on the S2 data products and tiling strategy is available on https://sentinel.esa.int/web/sentinel/missions/sentinel-2/data-products. Detailed information on the S2 L1C data products can be found in Gatti et al. (2018) [RD1].

2.2. Ancillary data and models

2.2.1. Geometric adjustment

Vector files are used for visual inspection of the quality of the geolocation of the S2 L1C input data. These shapefiles consist of easily recognisable features in the satellite imagery. When deviations larger than five meter are found, a shift is performed on the data. Table 2.1 lists the number of shapefiles within the different processed tiled used for geometric improvement. Figure 2.2 gives an example of a shapefile used for the determination of shift coefficients.

Table 2.1: Number of geometric features in each tile used for the geometric correction

Tile	31EUR	31UDS	31UES	31UET	31UFQ	31UFR	31UFS	31UFT
N°	3	4	4	7	4	4	4	7
Tile	31UFU	31UGR	31UGS	31UGT	31UGU	33UUA	33UVA	33UVV
N°	4	3	3	4	4	4	3	4

Figure 2.2: Example of easy recognizable feature used for geometric correction present in Tile 31UES.

More information on the implementation is given in Section 4.1 Geometric adjustment.

2.2.2. Pixel classification

Pixel classification in the Terrascope workflow is performed using the standalone version for Linux of **Sen2Cor v2.5.5** [RD2], (release date: 19/03/2018). The SceneClass Module is used to generate the Scene classification layer and subsequently also the Cloud and Shadow Masks. In order to generate this Scene classification, Sen2cor v2.5.5 is now also able to use the surfaces of the **Climate Change Initiative (CCI)** Land Cover data from 2015 (v2.0.7) as auxiliary information [RD2]. This is a package of 24 annual global land cover maps, at a resolution of 300m, spanning a twenty-four year period from 1992-2016. These land cover maps were produced through state-of-the art reprocessing of the NOAA-AVHRR HRPT, SPOT-Vegetation, ENVISAT-MERIS FR and RR, ENVISAT-ASAR and PROBA-V archives. The use of this auxiliary CCI information is not yet implemented in Terrascope v102 workflow, but will be included in the next version.

More information on the implementation is given in Section 4.2 Pixel classification.

2.2.3. Atmospheric Correction

The atmospheric correction algorithm makes use of following ancillary data:

- **Image correction for atmospheric effects (iCOR) [RD3]**
  The Terrascope workflow uses iCOR (release date: 18/08/2017) to perform an atmospheric correction. iCOR relies on Moderate Resolution Atmospheric Transmission Model-5 (MODTRAN5) for the radiative transfer modelling (Berk et al. 2006). The implementation of iCOR is described in detail in Section 4.3.

- **MODTRAN5 Look-Up-Tables (LUT)**
  iCOR relies on pre-calculated LUT tables based on MODTRAN5 radiative transfer modelling (Berk et al., 2006). These LUTs yield atmospheric correction parameters and diffuse transmissions in function of view zenith angle (VZA), solar zenith angle (SZA), relative azimuth angle (RAA), Aerosol Optical Thickness (AOT) and elevation. The parameters used to generate this LUT are explained in ANNEX I – MODTRAN5 LUT input parameters.

- **Digital Elevation Model (DEM)**
  The Global Land One-km Base Elevation (GLOBE) is a 30-arc-second (+/- 1 km) gridded, quality-controlled global DEM. The data is projected in Lat/Lon WGS84 at a scale of 0.008333 degrees or +/- 1km (Hastings et al. 1999). Figure 2.3 displays GLOBE.

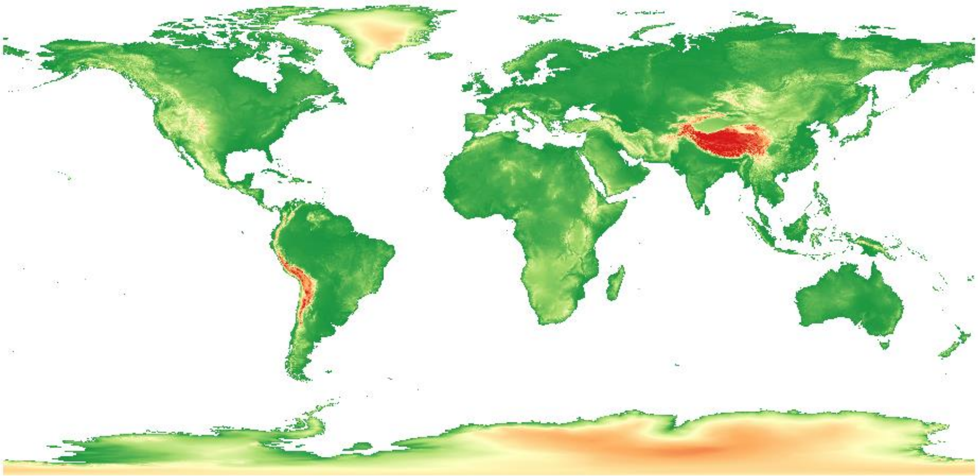


Figure 2.3: GLOBE DEM (Hastings et al., 1999)

- **Angle information**
  The angle information, i.e. Solar Zenith Angle (SZA), View Zenith Angles (VZA) and Relative Azimuth Angles (RAA), are obtained from the S2 L1C metadata.

  In the S2 L1C products, the angles are provided at 5000 meters resolution by detector. The solar angles (SZA and Sun Azimuth Angle (SAA)) given in the metadata eXtensible Markup Language (XML) file are resampled to 10, 20 and 60m. The detector dependency hamper such a simple resampling for the viewing angles (VZA and View Azimuth Angle (VAA)): the detector footprints overlap in the limit of each detector, and in older formats of S2 it is not possible to determine exactly from which detector a pixel of the overlap area originates. Consequently, mean viewing angle values are used for a whole tile.

  On 06/11/2018 ESA deployed a new Production Baseline (02.07) which includes an accurate detector footprint. With this information it is possible to link one pixel to one detector. This information is not implemented in Terrascope v102 workflow, but will be included in the next version.

- **Solar Irradiance**
  The solar spectral irradiance dataset from Thuillier et al. (2003) is used in the Terrascope atmospheric correction. This dataset covers a spectral range from 200 to 2400 nm, measured by the SOLar SPECtrum (SOLSPEC) spectrometer from the Atmospheric Laboratory for Applications and Science (ATLAS) and European Retrieval CArrier (EURECA) missions.

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

- **Spectral endmembers**

iCOR includes a land-based Aerosol Optical Thickness (AOT) retrieval technique, which describes the surface by a linear combination of three pure vegetation spectra and one soil spectrum. The spectral signatures of these four endmembers are presented in Figure 2.4.

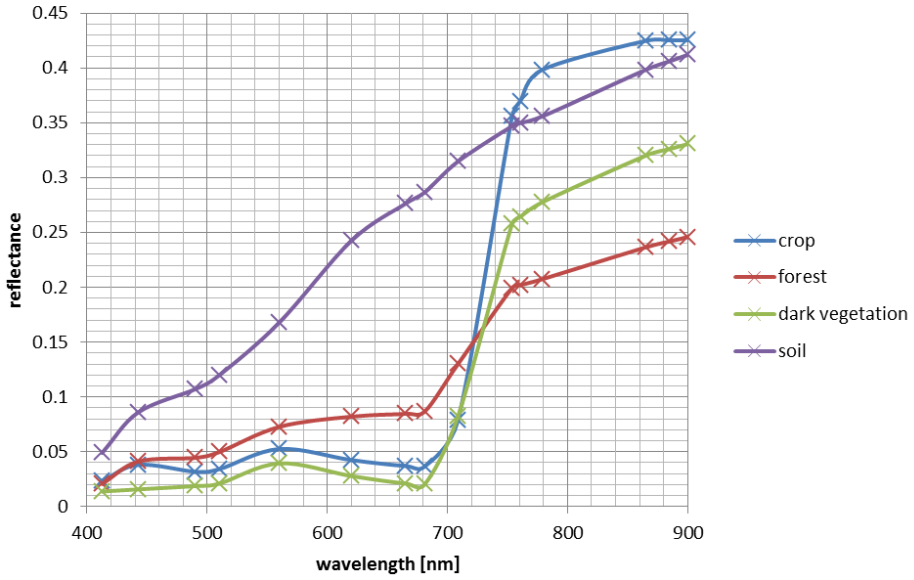


Figure 2.4 Spectral reflectance of the four endmembers used in the iCOR land-based AOT retrieval

- **AOT fall-back datasets**
  An AOT fall back mechanism is implemented in case the image doesn't allow an accurate AOT retrieval (see Section 4.3.2 Implementation). This fall back mechanism relies on external AOT data from the Copernicus Atmospheric Monitoring Service (CAMS):
  - Near-Real Time (NRT) AOT values at 550 nm - http://apps.ecmwf.int/datasets/data/cams-nrealtime/levtype=sfc/ (Morcrette et al, 2009)
  - Climato monthly AOT averages at 550 nm (Inness et al., in review)

3. Output

3.1.1. Product layers

The S2 TOC products generated and distributed by Terrascope include several files which are the output of the iCOR processor for the atmospheric correction and of the Sen2Cor processor for the masks (Cloud/Shadow) and the Scene Classification. The output file format is a single layer compressed Geostationary Earth Orbit Tagged Image File Format (GeoTIFF). Figure 3.1 shows the S2 TOC product file list.

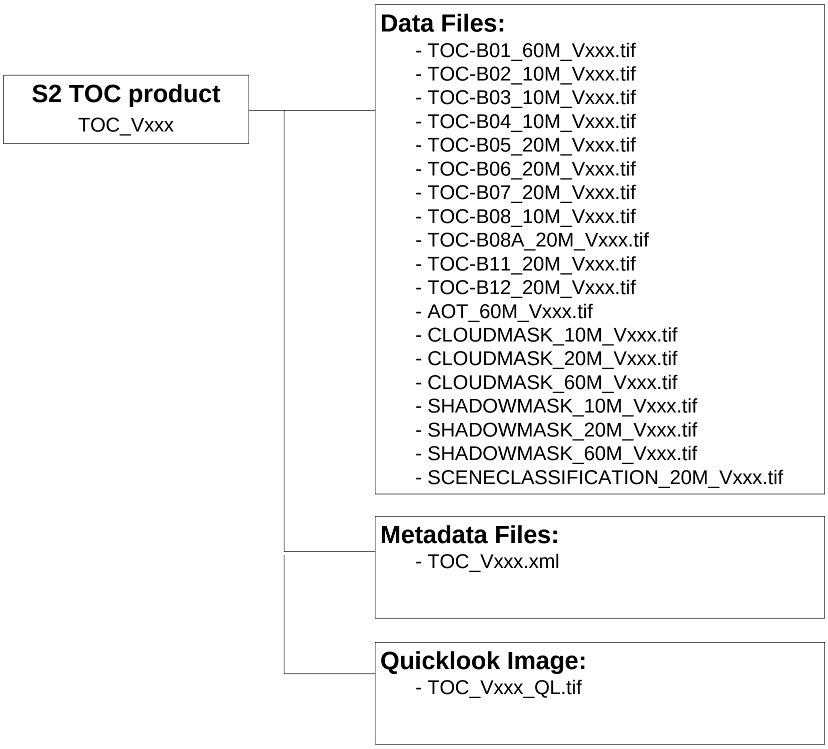


Figure 3.1: S2 TOC product file list

The S2 TOC Spectral Bands span from the visible and the Near Infra-Red to the Short Wave Infra-Red in different resolutions. The spatial and spectral characteristics are listed in Table 3.1. Note that B09 and B10 are not delivered as these contain respectively the water vapor and cirrus bands.

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

Layer	Spatial resolution (m)	S2A		S2B	
		Central wavelength (nm)	Bandwidth (nm)	Central wavelength (nm)	Bandwidth (nm)
TOC-B01_60M	60	443.9	27	442.3	45
TOC-B02_10M	10	496.6	98	492.1	98
TOC-B03_10M	10	560.0	45	559.0	46
TOC-B04_10M	10	664.5	38	665.0	39
TOC-B05_20M	20	703.9	19	703.8	20
TOC-B06_20M	20	740.2	18	739.1	18
TOC-B07_20M	20	782.5	28	779.7	28
TOC-B08_10M	10	835.1	145	833.0	133
TOC-B8a_20M	20	864.8	33	864.0	32
TOC-B11_20M	20	1613.7	143	1610.4	141
TOC-B12_20M	20	2202.4	242	2185.7	238

The AOT is provided in the native 60m resolution.

The physical pixel values in the S2 TOC files are converted from floating point values into integers, mainly to reduce the size of the files. Table 3.2 lists the technical information of the S2 TOC product with information necessary to calculate the physical values from the digital numbers available in the files. The physical number can be defined by using the following formula:

Physical Number = Scaling * Digital Number + offset.

Table 3.2: Technical information on the S2 TOC and AOT values

Technical information on the S2 TOC values		AOT
Physical min	-1.0	0.00
Physical max	1.0	2.5
Digital number min	-10000	0
Digital number max	20000	250
Scaling	1/10000	1/10000
Offset	0.0	0.0

The scene classification module allows to detect clouds, snow and cloud shadows and to generate a classification map, which consists of 4 different classes for clouds (including cirrus), together with six classifications for shadows, cloud shadows, vegetation, soil / desserts, water and snow.

The output of the Sen2Cor processing step in Terrascope is the Scene Classification at 20 m and derived cloud/shadow masks at three resolutions (*_10M, *_20M, *_60M). These cloud/shadow masks are derived by reclassifying and resampling the Scene classification layer as specified in Section 4.2. The values of the pixel classification layers are specified as shown in Table 3.3. [RD2]

Table 3.3: Explanation of pixel classification values

Layer	Value	Classification
CLOUDMASK	0	NO_CLOUD
	1	CLOUD
SHADOWMASK	0	NO_SHADOW
	1	SHADOW
SCENE CLASSIFICATION	0	NO_DATA
	1	SATURATED_OR_DEFECTIVE
	2	DARK_AREA_PIXELS
	3	CLOUD_SHADOWS
	4	VEGETATION
	5	BARE_SOIL
	6	WATER
	7	UNCLASSIFIED
	8	CLOUD_MEDIUM_PROBABILITY
	9	CLOUD_HIGH_PROBABILITY
	10	THIN_CIRRUS
	11	SNOW

3.1.2. Product version

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

- X is 0 during prototyping and pre-operational use. X is 1 for the first operational setup, and increments when if its results are no longer backward compatible (i.e. any further processing will have to be adapted to deal with e.g. format changes, value scaling, …).

- Y is reset to 0 with an X increment. Y increments when functionality is added, but backward compatibility is guaranteed (e.g. when a different approach is taken for atmospheric or geometric correction.

- Z is reset to 0 when Y increments. Z increments when the software is patched (bug fixed) without any functional changes.

The current version of the Terrascope Sentinel2 workflow is v102.

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

3.1.3. Product data access

The Terrascope S2 data products can be accessed through:

- Terrascope website: https://terrascope.be/en
  For viewing, discovery and data access.

- VITO Product Distribution Portal (PDP) : http://www.vito-eodata.be/
  Catalogue with download possibility.

- PROBA-V Mission Exploitation Platform (MEP) : https://proba-v-mep.esa.int/
  For expert users to develop processing on demand tools or use the data within the virtual research environment.

The details of each of these access points are described in detail in the Terrascope Sentinel-2 Products User Manual (Paepen et al. 2019) [RD4].

4. Methodology

4.1. Geometric adjustment

4.1.1. Justification

The L1C product provided by ESA and used as input in the Terrascope workflow, is geometrically corrected and results from using a DEM to orthorectify the image (Gascon, 2014). Nevertheless, on some occasions a geometric shift was noted in the products. An exceptional example was a shift of +/- 50 m noted on 16/08/2016, as illustrated in Figure 4.1.

Figure 4.1 Geometric shift noted on 16/08/2016 in tile T31UFS.

Terrascope performs an adjustment step to guarantee a minimal geometric shift between multi-temporal images for the Belgian users. The first validation results of this assessment are included in Section 6.2

4.1.2. Implementation

The geolocation of the S2 data is visually inspected by an operator using vector files with a set of control points, consisting of 4 to 7 easily recognizable features per image (100 x 100 km²). When the average deviation from the control points is larger than five meters in the x and/or y direction, a correction is applied: a linear shift is performed on the image in the x and/or y direction equal to the average deviation calculated for all control points.

4.1.3. Outlook

ESA is implementing a geometric refinement step to meet the multi-temporal geolocation requirement (<0.3 pixel at 95%) in the L1C products (Clerc et al. 2019). When this refinement step is implemented, we will validate the results and check whether the Terrascope adjustment step can be skipped.

4.2. Pixel classification

4.2.1. Justification

Including a pixel classification in the output, facilitates the exploitation of the TOC products in further processing steps. A couple of well-known tools exists, including Sen2Cor (Mueller-Wilm et al, 2018) [RD2] and Fmask (Zhu et al., 2015). Based on a quality assessment study, see Section 6.3, it was decided to include Sen2Cor v2.5.5 in the Terrascope workflow.

4.2.2. Implementation

Sen2Cor 2.5 is a processor for Sentinel-2 Level2 product generation and formatting; it performs the atmospheric, terrain and cirrus correction of Top-Of Atmosphere L1C input products. This Sen2Cor processor is freely available online from the ESA STEP (Science toolbox exploitation platform) portal. More information on this processor can be found at http://step.esa.int/main/third-party-plugins-2/sen2cor/. [RD2]

Sen2Cor consists of two important processing modules, the SceneClass Module and the AtmCorr Module. In the Terrascope workflow, only the SceneClass Module is implemented. This module allows to detect clouds, snow and cloud shadows and to generate a classification map (so-called scene classification) including also information on dark areas, vegetation, bare soil , water and snow.

Sen2Cor v2.5.5 is able to use the surfaces of the Climate Change Initiative (CCI) Land Cover data from 2015 as auxiliary information. This is used in Sen2Cor to improve the accuracy of Sen2Cor classification over water, urban and bare areas and also to have a better handling of false detection of snow pixels. [RD2] . The use of this auxiliary CCI information is not yet implemented in the Terrascope v102 workflow, but will be included in the next version.

Based on the Sen2Cor classification, two additional mask layers are created and made available to the users:

- CLOUDMASK: If the pixel was either classified by Sen2Cor as CLOUD_MEDIUM_PROBABILITY or CLOUD_HIGH_PROBABILITY

- SHADOWMASK: If the pixel was classified as CLOUD_SHADOWS

4.2.3. Outlook

Future updates of the Sen2Cor SceneClass module will be evaluated. If the updated version results in a significant improvement, the Terrascope workflow will be updated to include the new version.

4.3. Atmospheric correction

4.3.1. Justification

When electromagnetic radiation passes through the atmosphere it may be transmitted, scattered or absorbed. Using S2 data for quantitative remote sensing of land or water surfaces requires the removal of atmospheric effects, which is essential to convert radiance measured by the sensors to surface reflectance. Hadjimitsis et al. (2010) argued that atmospheric correction is the most important part of the pre-processing of satellite remotely sensed data. For agricultural applications, any omission of considering the effects of the atmosphere when vegetation indices from satellite images are used, may lead to major discrepancies in the final outcomes. For example neglecting atmospheric correction when calculating Normalized Difference Vegetation Index (NDVI), a widely used index in agricultural studies, will result in an average error of 18 % and the outcomes are then no longer useful for e.g. crop growth monitoring.

The Terrascope chain uses the iCOR atmospheric correction method (De Keukelaere et al., 2018) [RD3]. iCOR has been involved in a couple of validation exercises , including the Atmospheric Correction Intercomparison Exercise (ACIX) organized by ESA-NASA (Doxani et al., 2018). These validation efforts will be continued in the ACIX-II exercise. Since August 2017, iCOR is also released to the broader user community as a plugin in the SNAP toolbox for Landsat-8 and Sentinel-2 data (https://blog.vito.be/remotesensing/icor_available). Since its release over 800 users worldwide downloaded the tool. A quality assessment of iCOR is given in Section 6.4.

The implementation of iCOR is chosen over SEN2COR because of the following reasons:

- It's applicability to other sensors, including Proba-V and Sentinel-3. This facilitates the combined use of TOC and derived products from different origins in later stages. https://remotesensing.vito.be/technology/atmospheric-correction-optical-sensors
- iCOR offers the option to use an external AOT source instead of deriving the information from the image itself. In the Terrascope workflow an AOT fall back mechanism is implemented, which allows operational processing.

4.3.2. Implementation

Figure 4.2 shows the flowchart of the atmospheric correction implemented in Terrascope. Starting from S2 TOA L1C products, an iCOR masking is applied yielding land/water and cloud intermediate layer files. In the next step, AOT values are either retrieved from the S2 image, or obtained from an external dataset, i.e. CAMS data (Morcrette et al., 2009 & Inness et al., in review). The land/water, cloud and AOT layers together with MODTRAN5 LUTs, DEM and the solar and viewing angles (mean of the angular values given in S2 metadata file) are used as input for the actual atmospheric correction with iCOR. The result is an S2 TOC product.

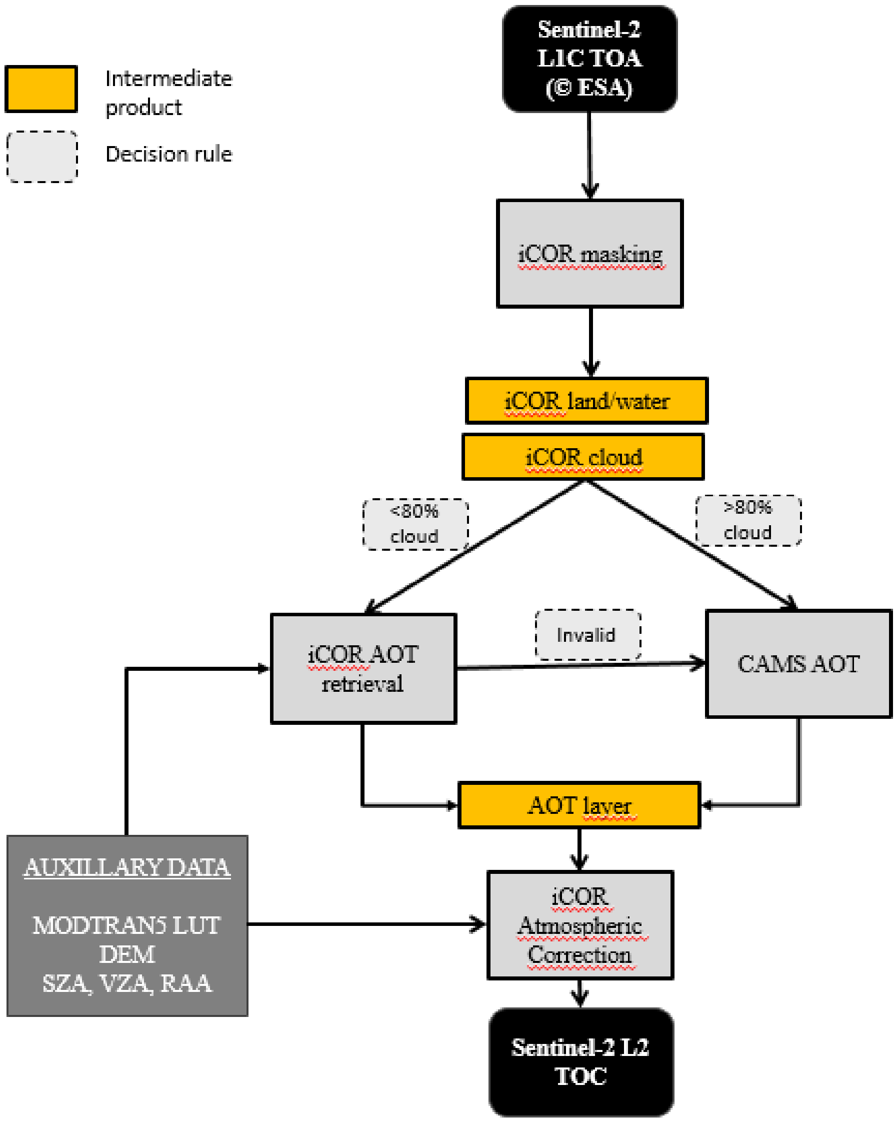


Figure 4.2: Workflow of iCOR implemented in the Terrascope processing chain. iCOR AOT retrieval is invalid when the absence of clear land pixels hamper an accurate image-based AOT retrieval.

Internal iCOR land/water mask

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

Internal iCOR cloud detection

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

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

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

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

AOT at 550 nm

The origin of the AOT data at 550 nm used in the atmospheric correction of the Terrascope products depends on the quality of the image: by default the AOT will be retrieved from the imagery using iCOR [RD3]. When the cloud percentage is too high (>80%) or the iCOR derived AOT product is invalid (not enough land or spectral variety) an external AOT dataset will be used. CAMS NRT data as provided by ECWMF are preferred, unless the time window between S2 and CAMS NRT data becomes too large (>24h). Such rare cases can happen when connection issues occur between the servers. In these cases, CAMS climato monthly averages (Inness et al., in review) are used. The fall back mechanism is depicted in Figure 4.3.

The iCOR image-based AOT retrieval subdivides the TOA image into blocks of about 15 x 15 km², large enough to include high spectral variation and small enough to assume spatial atmospheric homogeneity. In a first step a max threshold on the AOT values is set using a dark dense vegetation approach. Next, the AOT value is refined using the spectral variation with the 15 x 15 km² block, using a multiparameter endmember inversion technique. Five pixels with high spectral contrast (selected based on the NDVI values from TOA reflectance) are represented by a linear combination of three pre-defined default vegetation spectra and a soil spectrum, see Section 2.2.3.

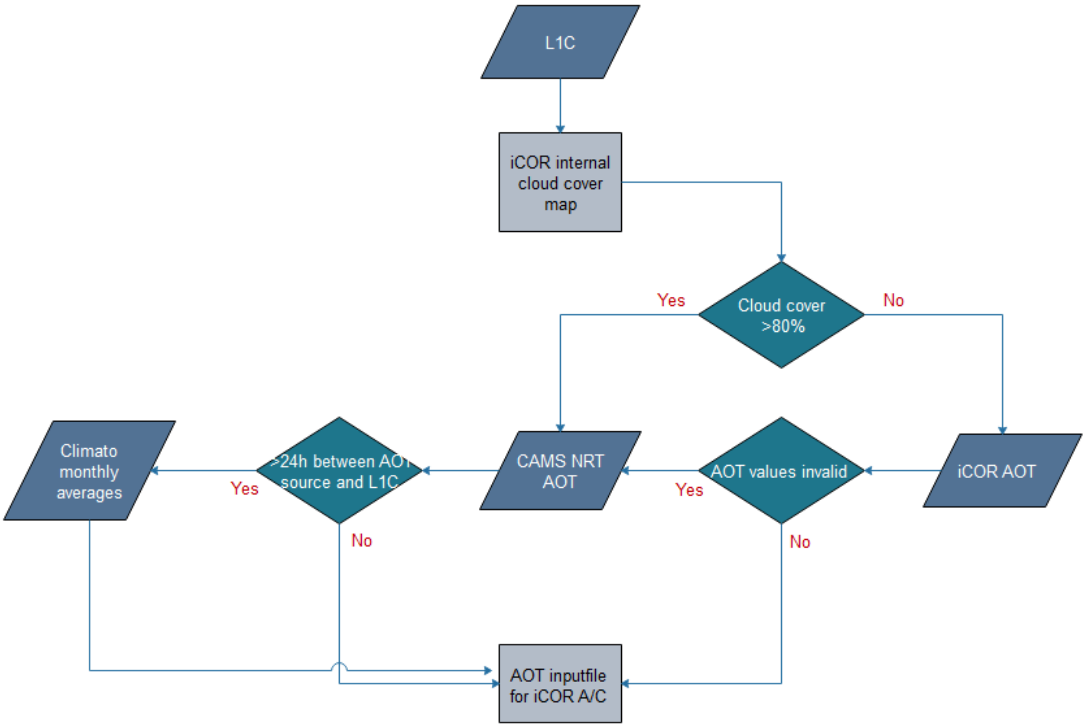


Figure 4.3: Flowchart explaining the AOT origin

iCOR Atmospheric correction

In the final step, all generated input data are inserted in the iCOR atmospheric correction. The water vapour is fixed at 2.0 g.cm^{-2} and the aerosol model is fixed at a continental model. The option for performing an adjacency correction is disabled in the Terrascope workflow, since the focus are land-based products where adjacency effects are less important. In Section 6.4 a first quality assessment of the iCOR atmospheric correction is included.

4.3.3. Outlook

The current iCOR implementation can show small discrepancies between neighbouring tiles, see Section 5.3. Since the CAMS NRT AOT and iCOR AOT data show good regression statistics, the next Terrascope version will use the CAMS NRT data as input in the atmospheric correction. The iCOR inherent land/water mask will be improved: water is very absorbing in the SWIR region. Therefor the next version will work with a SWIR band at 20 m instead of the 842 nm band at 10 m to create an internal land/water mask.

5. Limitations

5.1. Geometric adjustment

The limitations for the current geometric adjustment step is the interactive step and the availability of easily recognizable features in shapefile format. This limits its applicability to worldwide processing. Since ESA is improving the L1C products, this step might become unnecessary in next versions of the Sentinel-2 Terrascope processing chain.

5.2. Pixel classification

Each new update in the Sen2Cor scene classification module will be analysed in terms of added value compared to previous versions and the required effort for implementation or update. Only if the cost/benefit analysis is positive, the update will be implemented.

5.3. Atmospheric correction

The current version of the iCOR atmospheric correction is tile based. Consequently, edge artefacts can occur between different tiles acquired on the same date. This is illustrated in Figure 2.1. These artefacts are most pronounced when in one tile the AOT is derived from the image itself, while in the neighbouring tile the AOT CAMS NRT fall back mechanism is activated. As mentioned in Section 4.3.3, the next version of Terrascope will use CAMS AOT only as input in iCOR. Besides solving the edge artefacts issues, shifting to CAMS AOT is a first step towards on-the-fly processing.

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

The absorbent behaviour of water vapour makes this parameter important in atmospheric processes. In the current workflow this parameter is fixed at 2 g. cm^{-2}. This estimation will have an impact on the derived products. Besides water vapour, also the angles considered in the Terrascope workflow are not ideal: an average value for all bands is taken for viewing and solar angles. S2 consists of different detectors mounted slightly different resulting in different viewing angles across the full image. In a next version of iCOR, both mentioned limitations will be tackled. The MODTRAN5 tables work with continental aerosol models. This is acceptable for the current processing regions of Terrascope, but will have a lower performance over e.g. desert-like regions.

6. Quality assessment

6.1. Terrascope Sentinel-2 v101 vs v102

A regression analysis of TOC values between v101 and v102 is performed for two tiles (31UES) and both S2 satellites (S2A and S2B). The regression analysis is performed on 10,000 random pixels selected within each image. The intercept, slope and coefficient of determination (R^2) values for year 2017 are depicted in Figure 6.1 (tile 31UES S2A) and Figure 6.3 (tile 31UES S2B).

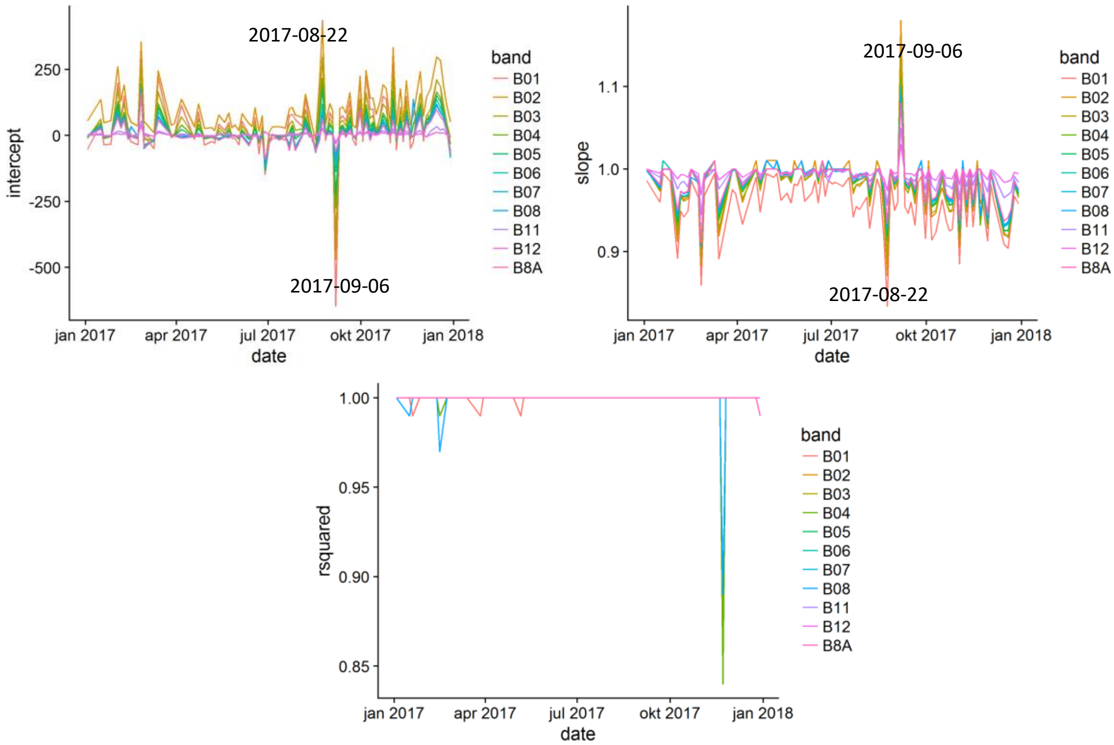


*Figure 6.1 Regression statistics between TOC products of V101 and V102 for 31UES – Sentinel-2A tiles. (top left) intercept (*10,000) (top right) slope and (bottom) the coefficient of determination (R^2) values for the different S2A spectral bands.*

The regression results for tile 31UES S2A show high R^2 values (> 0.83). Two outliers were detected: day 2017-08-24 and 2017-09-06. Figure 6.2 shows the quick looks of both images, which appear to be highly affected by clouds. In both cases the CAMS NRT fall back mechanism was triggered. This mechanism was not implemented in v101, hence the difference.

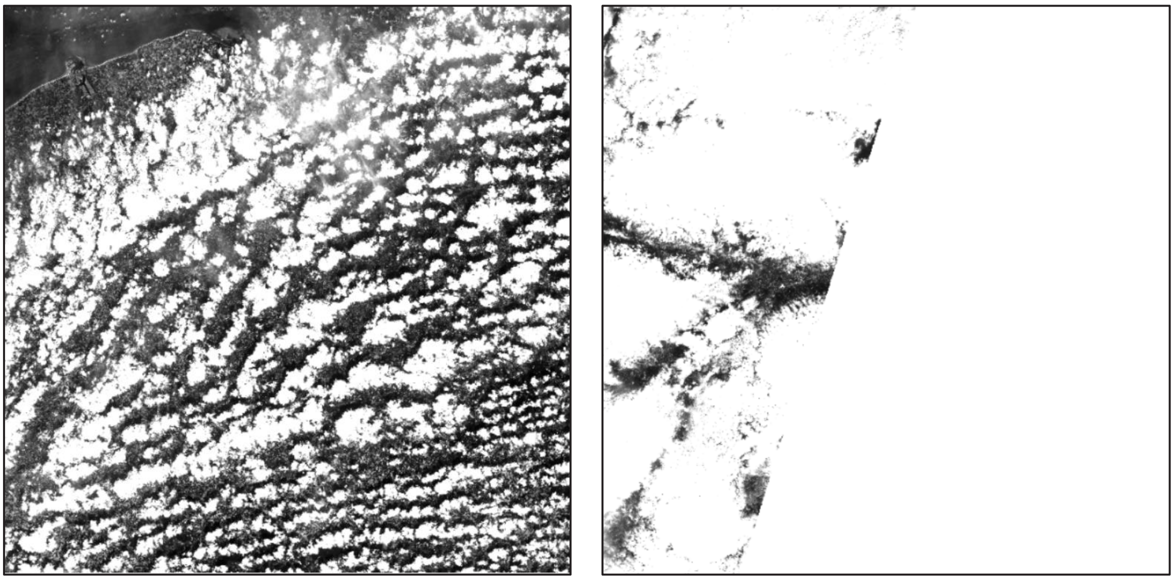


Figure 6.2 Quicklooks of tile 31UES S2A acquired on (left) 24-08-2017 and (right) 06-09-2017.

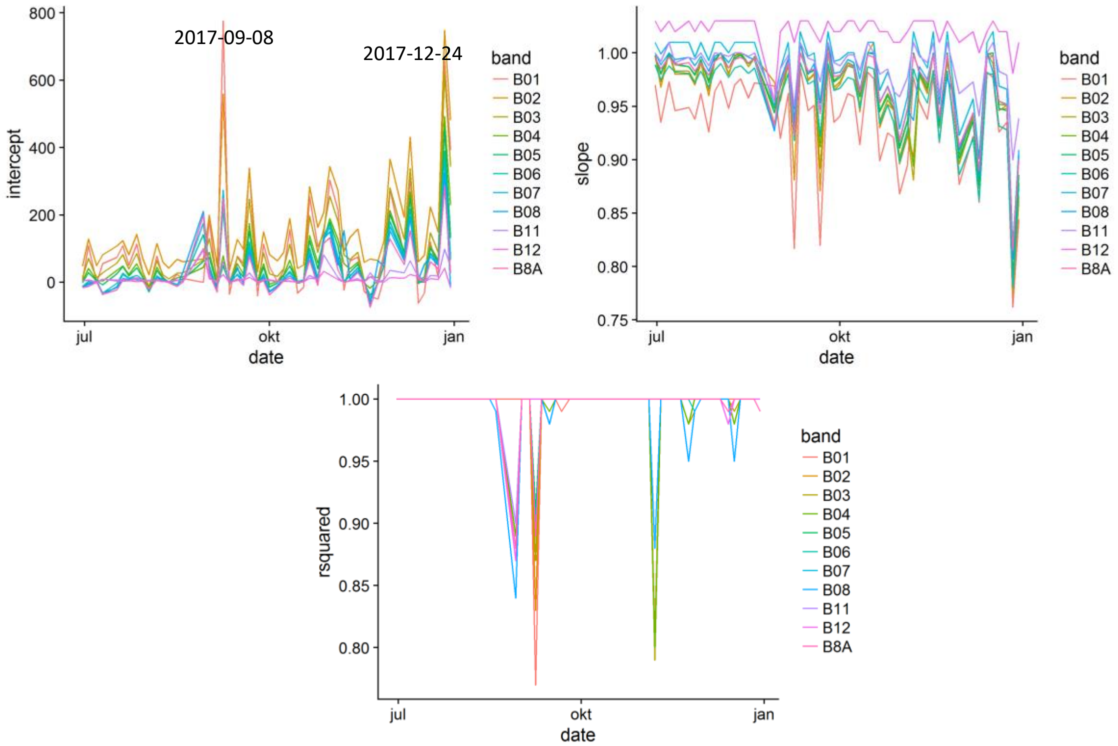


*Figure 6.3 Regression statistics between TOC products of V101 and V102 for 31UES – Sentinel-2B tiles. (top left) intercept (*10000) (top right) slope and (bottom) the coefficient of determination (R^2) values for the different S2A spectral bands.*

Larger changes of the same tile (31UES) but acquired with S2B are observed compared to S2A. This is because the V102 includes a separate S2B SRF, while in V101 the S2A SRF for both satellites was used. The two outliers (2017-09-08 and 2017-12-24) are related to triggering of the AOT fall back mechanism.

6.2. Geometric adjustment

Figure 6.4 shows the geometric shift parameters applied to the Sentinel-2 tiles, which are the result of the geometric adjustment step (see Section 4.1). The left graph in Figure 6.4 indicates a few outliers, including day 16/08/2016 where a shift of 45 m was found and applied. Also for 4/09/2015 and 30/06/2017 large geometric shifts (>30 m) where observed and applied. However, the standard deviation between the different individual shifts noted for each shapefiles within the tile is relatively large (> 50 m). These shifts were influence by cloudy conditions.

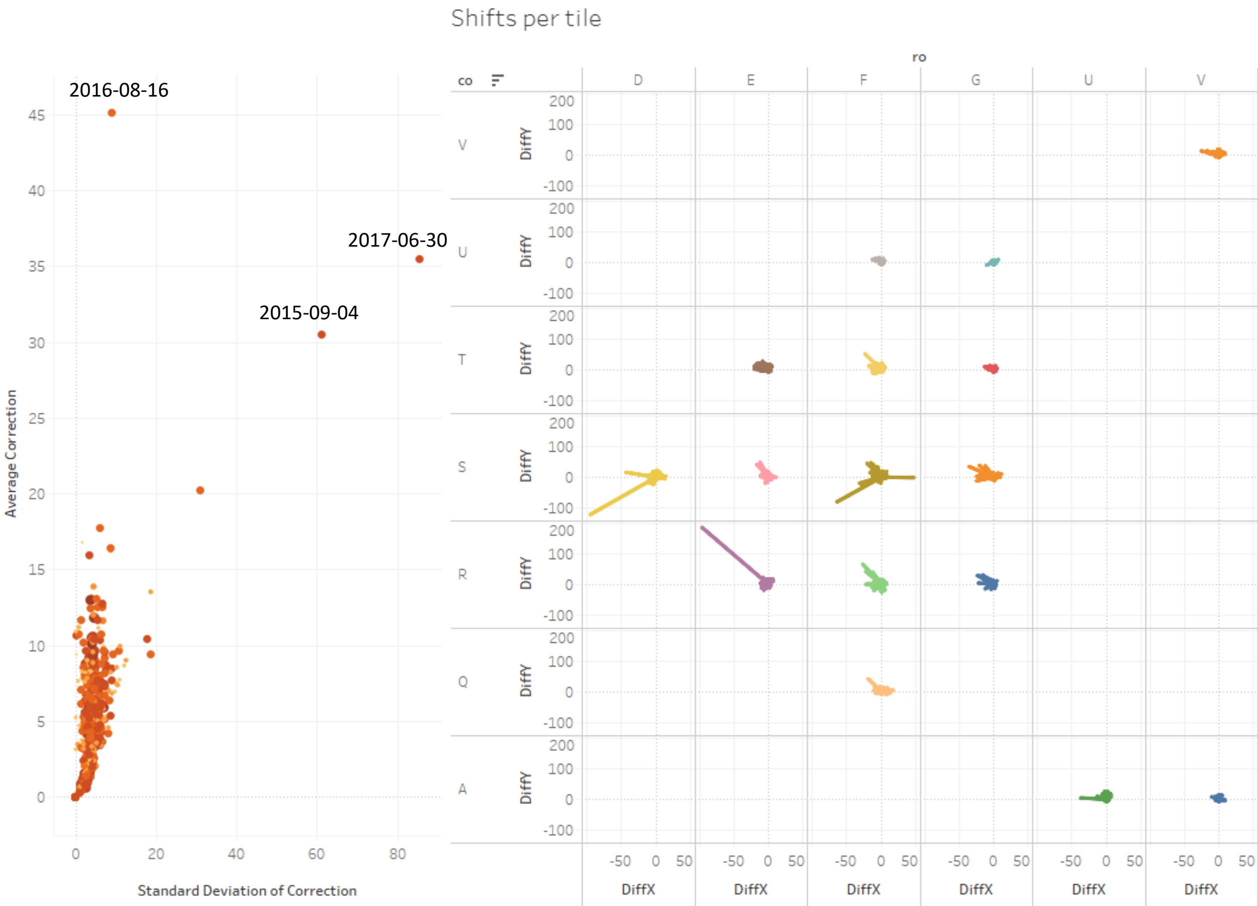


Figure 6.4 Geometric shifts of the S2 data. (l) The final shift parameter, expressed in meter, applied for each tile and the corresponding standard deviation noted within one tile. (r) Detention into the Individual shift parameters noted for each shapefile, expressed in meter for the two spatial dimensions.

6.3. Pixel classification

A quality assessment between different existing pixel classification tools was made before it was decided to include Sen2Cor 2.5 in the Terrascope chain. The investigated tools were: Sen2Cor v2.5, Sen2Cor v2.4, Fmask v40 and PythonFmask (http://pythonfmask.org/en/latest/ & https://github.com/gersl/fmask).

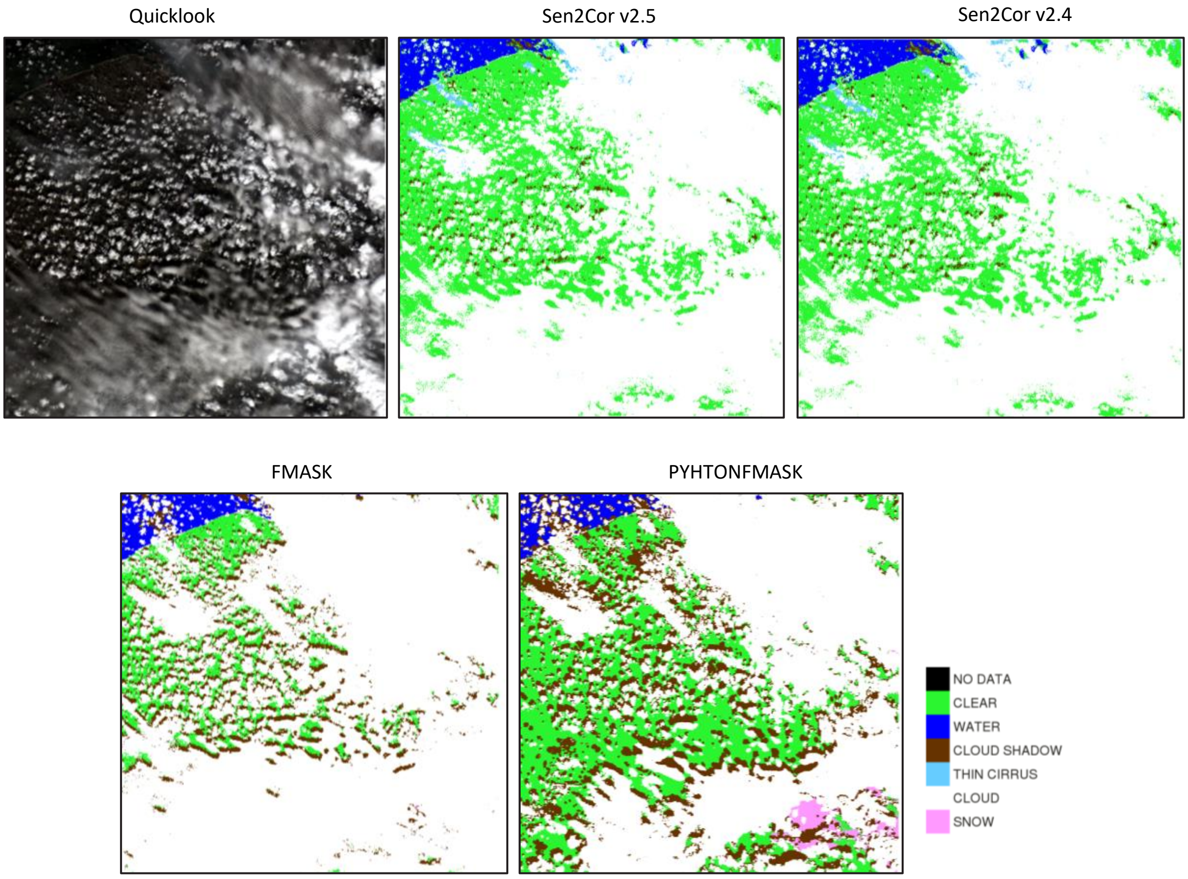


Figure 6.5 Results of different pixel classification tools for tile 31UES acquired on 16/04/2017

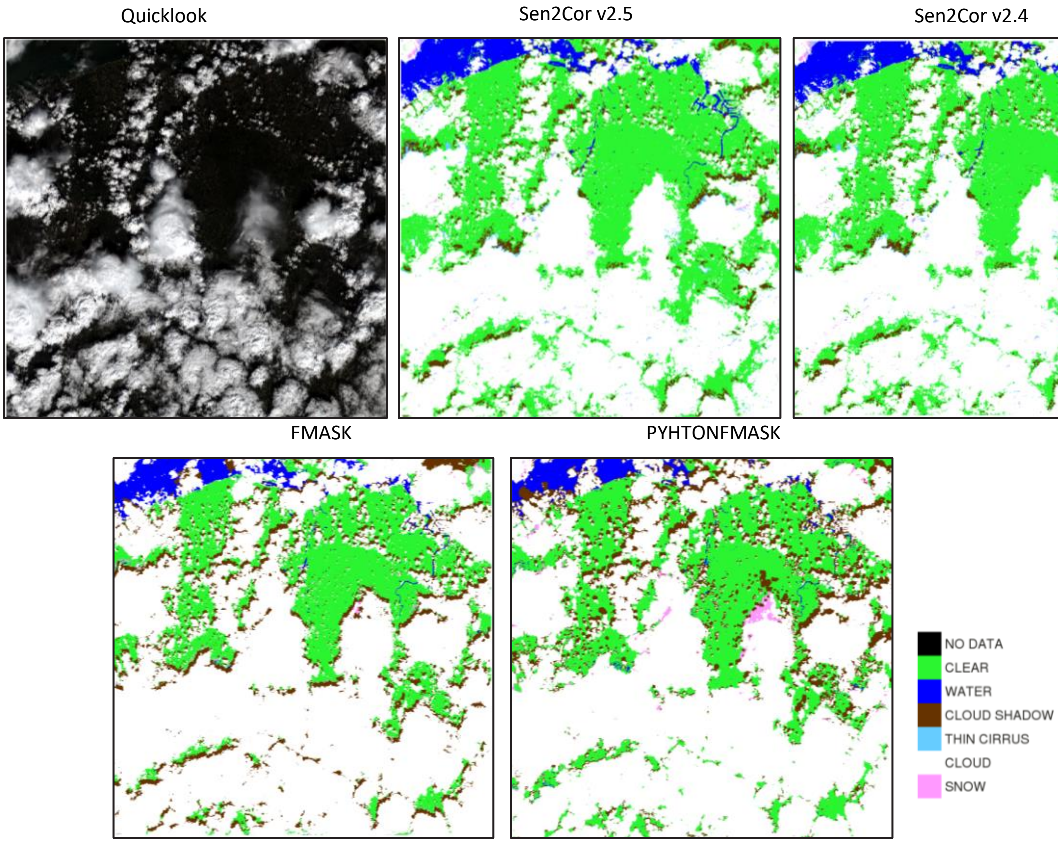
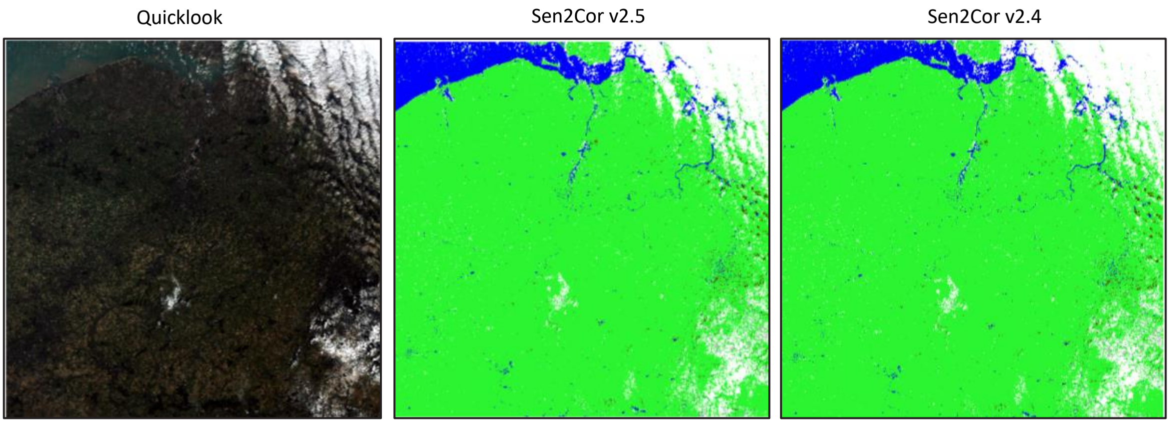


Figure 6.6 Results of different pixel classification tools for tile 31UES acquired on 26/04/2017



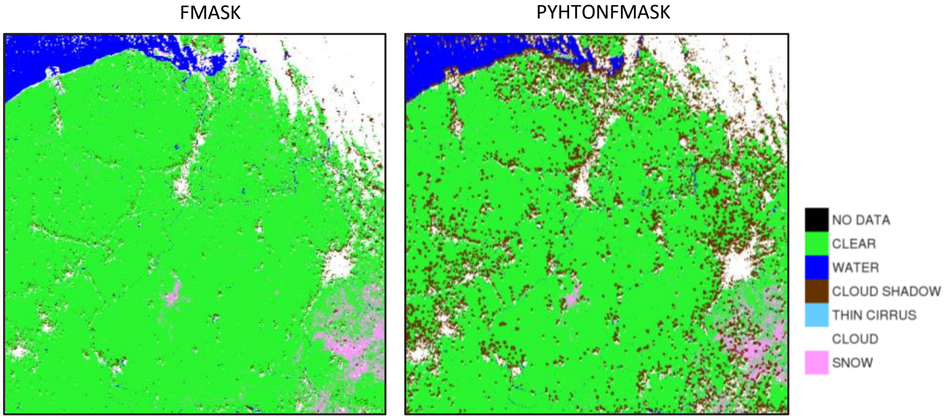


Figure 6.7 Results of different pixel classification tools for tile 31UES acquired on 26/01/2017

6.4. Atmospheric correction - AOT

The iCOR atmospheric correction has been involved in a couple of validation exercises , including the international Atmospheric Correction Intercomparison Exercise (ACIX) organized by ESA-NASA (Doxani et al., 2018). As most of the atmospheric correction methods that can be applied on S2 are participating in ACIX, it is considered as a peer-reviewed validation of iCOR. These validation efforts will be continued in the ACIX-II exercise.

This section reports on the quality assessment of the AOT used in the Terrascope workflow. Twenty-one different S2 tiles across the world were processed from 01/2017 – 09/2018. The location of the tiles are presented in Figure 6.8. Within these tiles an AERONET station was present, allowing a validation of the AOT at 550 nm. The tiles were selected to include a large variety of land cover types, listed in Table 6.1. Also seven AERONET-OC stations were included. These stations also record the normalized water-leaving radiance.

Figure 6.8 Distribution of the processed S2 tiles across the world. The tiles are marked with red dots.

Table 6.1 List of Sentinel-2 processed, the corresponding AERONET(-OC) station and the main land cover type.

Id	S2 Tile	Ocean Colour	Aeronet station(s)	Country	Characteristic
1	31UET		The_hague	Belgium	
2	31UFT		Cabauw	Belgium	
3	31UES	Yes (Zeebrugge)	Lille, Brussels, Zeebrugge	Belgium	
4	31UDS		Dunkerque	Belgium	
5	36RXV		SEDE_BOKER	Israel	Arid
6	31PDR		Banizoumbou	Niger	Arid
7	31PDQ		Banizoumbou	Niger	Arid
8	21LWK		Alta_Floresta	Brazil	Equatorial Forest
9	11TMM		Rimrock	USA	Boreal
10	11TNM		Rimrock	USA	Boreal
11	50TMK		Beijing	China	Temperate
12	55HFA		Canberra	Australia	Temperate
13	55HFB		Canberra	Australia	Temperate
14	35JPM		Pretoria_CSIR-DPSS	South-Africa	Temperate
15	32TQR	Yes	Venise	Italy (2 UTM zones!)	Coastal
16	33TUL	Yes	Venise	Italy (2 UTM zones!)	Coastal
17	35TPK	Yes	Gloria	Romenia	Coastal
18	32TPR	Yes	Sirmione	Italy	Mountain lake
19	31TFJ	Yes	Frioul	France	Coastal
20	31TFH	Yes	Frioul	France	Coastal
21	31UDT	Yes	Thornton C-Power	Belgium	Coastal

5045 Sentinel-2 tiles were processed for this validation exercise from 01-2017 till 09-2018. Out of this exercise, following results were obtained:

- In 45.49% the AOT fall back was triggered, reason:
  - 74.03 % cloud percentage > 80%
  - 25.97 % cloud percentage < 80%, but iCOR was not able to retrieve valid AOT values

    Sites:

Alta_Floresta	13
Banizoumbou	3
Beijing	6
Brussels	39
Cabauw	39
Canberra	15
Dunkerque	25
Frioul	87
Gloria	54
Lille	39
Pretoria_CSIR-DPSS	25
Rimrock	26
SEDE_BOKER	18
Sirmione_Musea_GC	5
The_Hague	34
Thornton_C-power	101
Venise	28
Zeebrugge-MOW1	39

Figure 6.9 shows the AOT validation of the current Terrascope workflow (iCOR with CAMS fallback) with AERONET AOT data. Pixels identified by iCOR as 'cloud' are disregarded in this analysis.

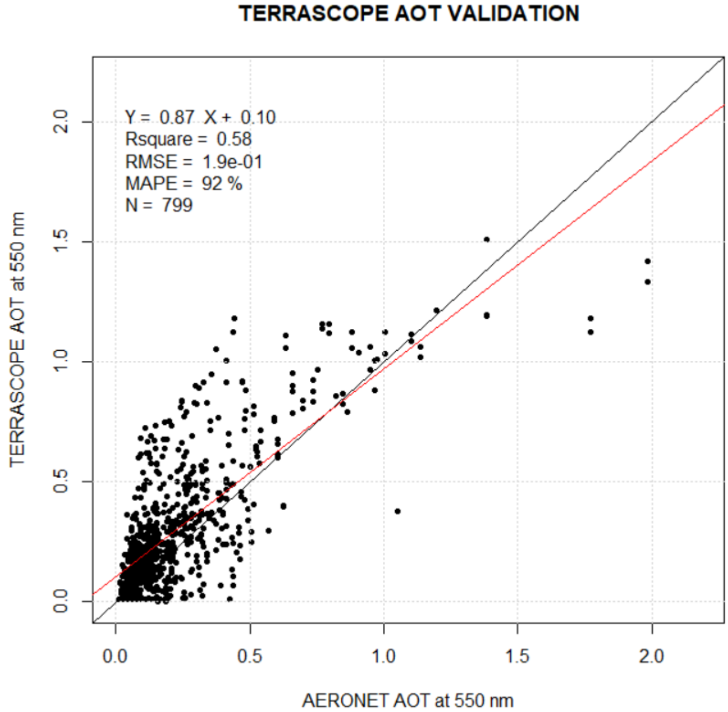


Figure 6.9 Terrascope AOT validation

Figure 6.10 and Figure 6.11 show the difference between the current Terrascope workflow and the land and water AERONET sites respectively. The water AERONET-OC stations are: Venice, Thornton_CPower, ZeebruggeMOW1 and Gloria. In 76 out of the 239 cases, the fall back was triggered for these water scenes.

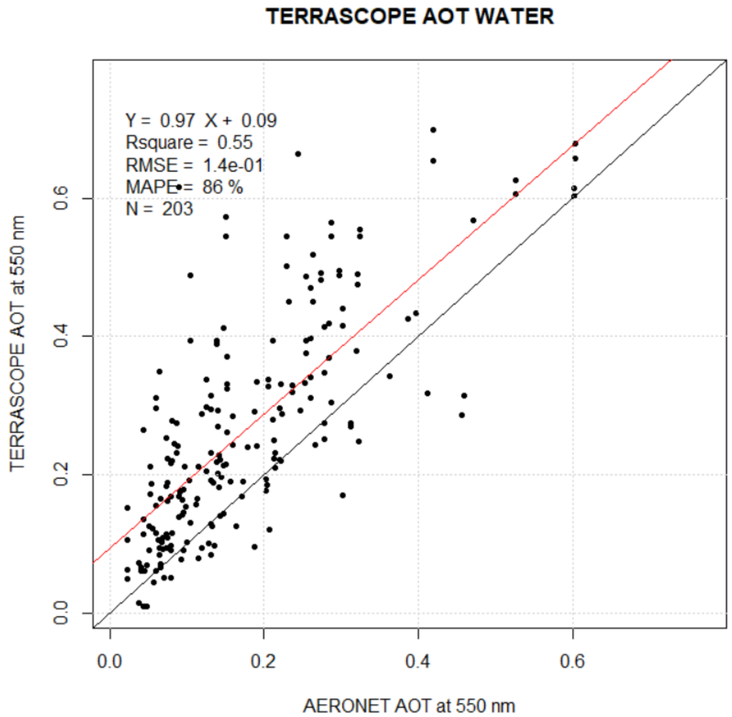


Figure 6.10 Terrascope AOT validation WATER

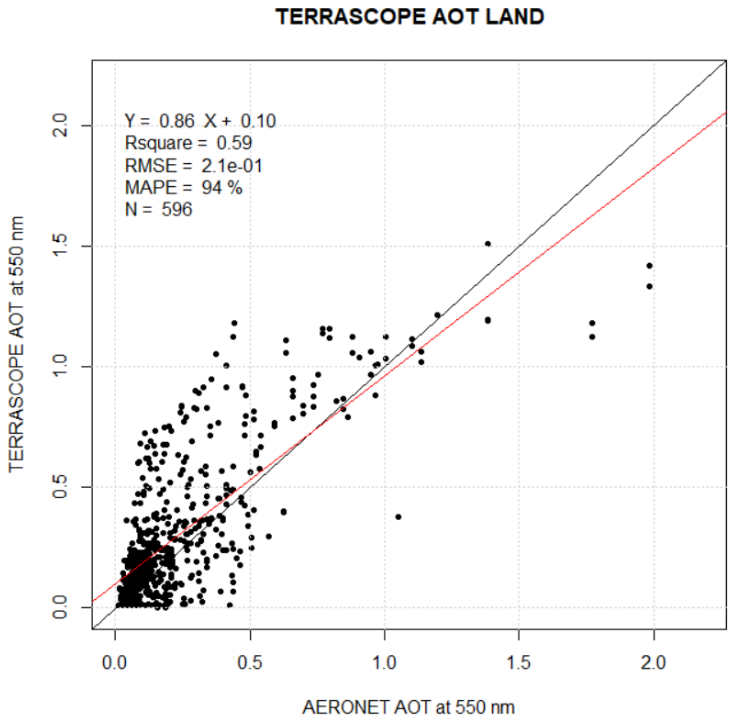
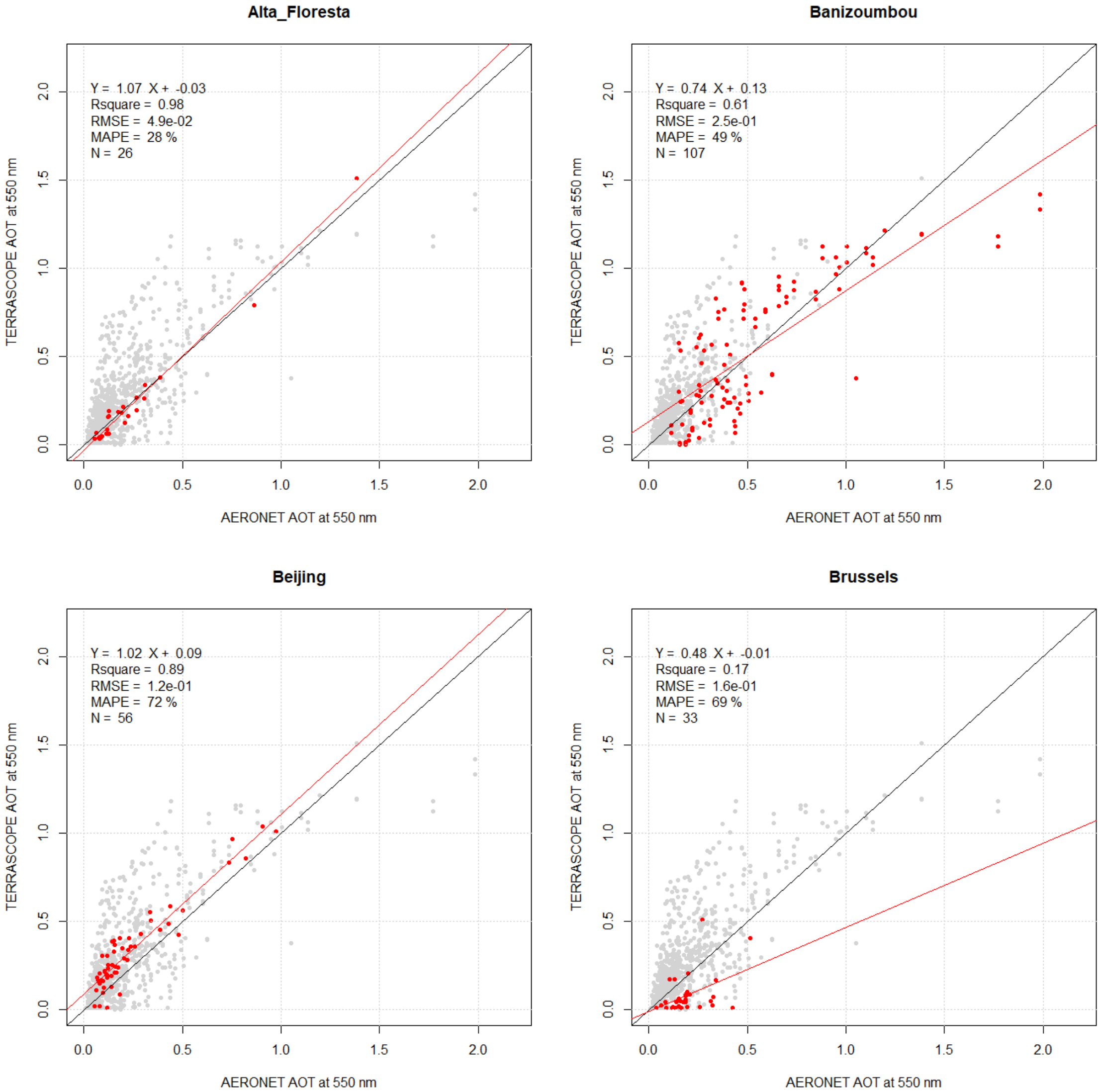
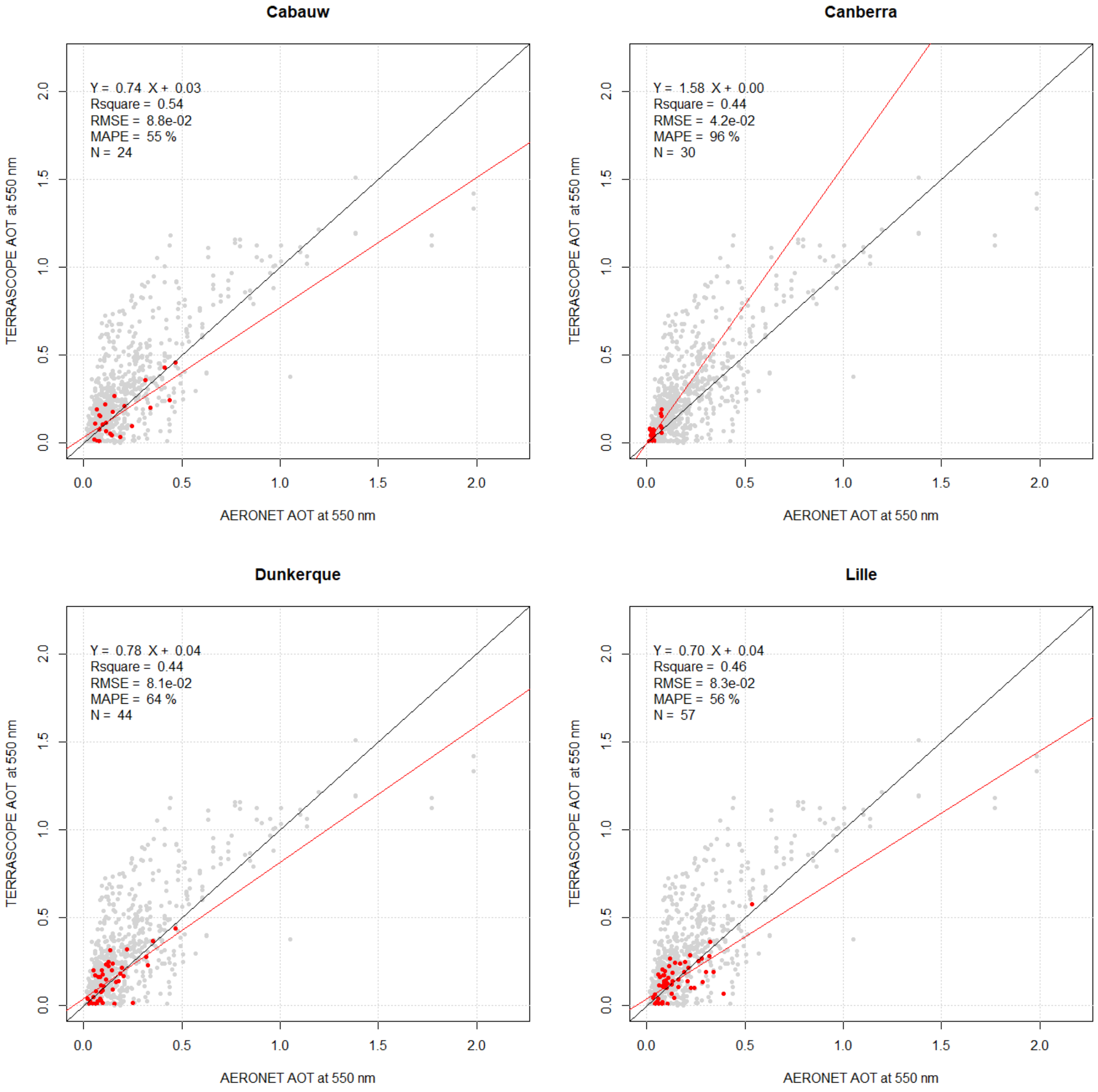
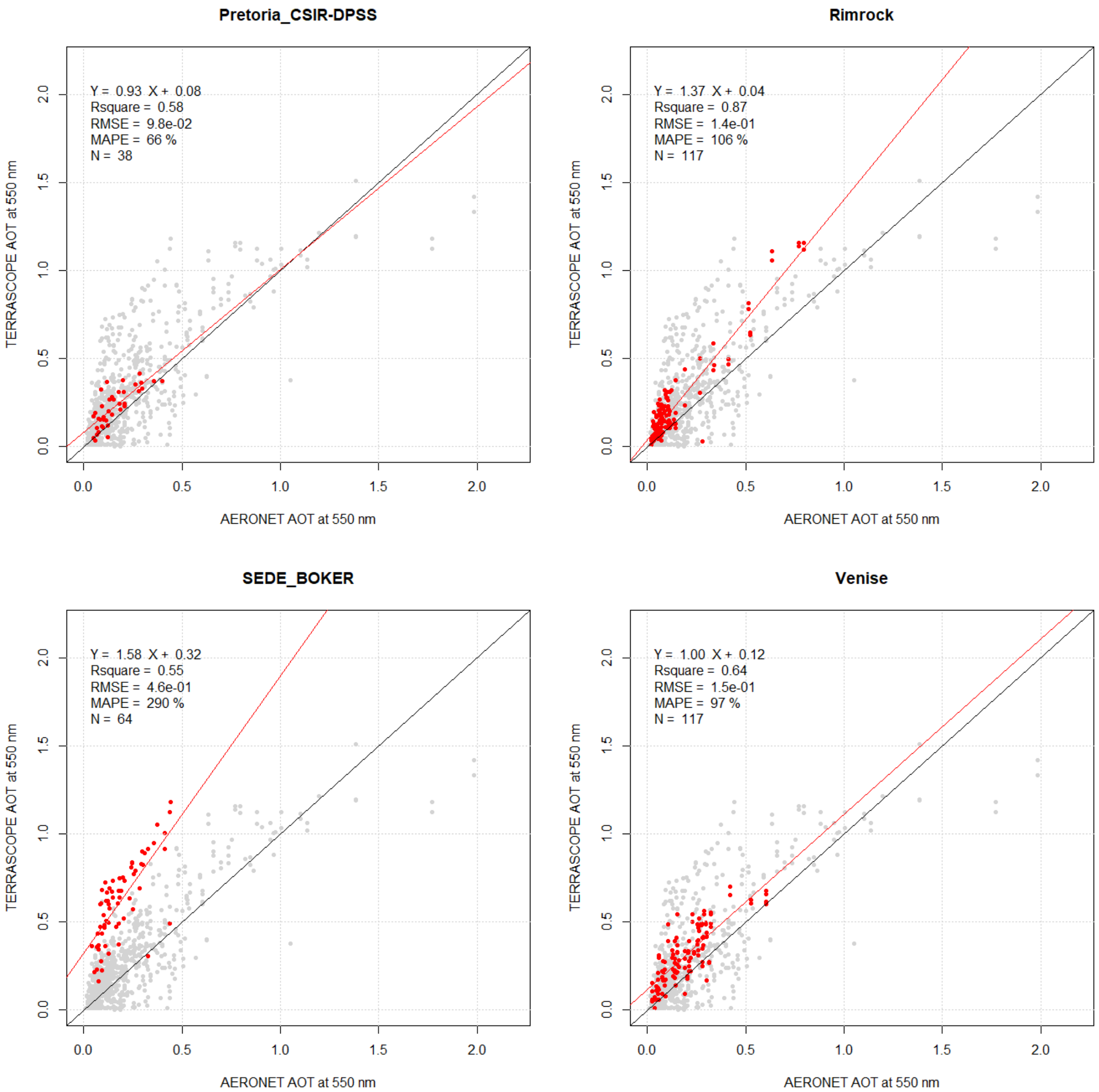


Figure 6.11 Terrascope AOT validation LAND

The next set of graphs (Figure 6.12) show the relation for the individual sites. The grey dots represent AOT values of the full dataset. The red dots are the values the mentioned site.




Cabauw
Y = 0.74 X + 0.03
Rsquare = 0.54
RMSE = 8.8e-02
MAPE = 55 %
N = 24
TERRASCOPE AOT at 550 nm
AERONET AOT at 550 nm
Canberra
Y = 1.58 X + 0.00
Rsquare = 0.44
RMSE = 4.2e-02
MAPE = 96 %
N = 30
TERRASCOPE AOT at 550 nm
AERONET AOT at 550 nm
Dunkerque
Y = 0.78 X + 0.04
Rsquare = 0.44
RMSE = 8.1e-02
MAPE = 64 %
N = 44
TERRASCOPE AOT at 550 nm
AERONET AOT at 550 nm
Lille
Y = 0.70 X + 0.04
Rsquare = 0.46
RMSE = 8.3e-02
MAPE = 56 %
N = 57
TERRASCOPE AOT at 550 nm
AERONET AOT at 550 nm


Pretoria_CSIR-DPSS
Y = 0.93 X + 0.08
Rsquare = 0.58
RMSE = 9.8e-02
MAPE = 66 %
N = 38
Rimrock
Y = 1.37 X + 0.04
Rsquare = 0.87
RMSE = 1.4e-01
MAPE = 106 %
N = 117
SEDE_BOKER
Y = 1.58 X + 0.32
Rsquare = 0.55
RMSE = 4.6e-01
MAPE = 290 %
N = 64
Venise
Y = 1.00 X + 0.12
Rsquare = 0.64
RMSE = 1.5e-01
MAPE = 97 %
N = 117
TERRASCOPE AOT at 550 nm
AERONET AOT at 550 nm

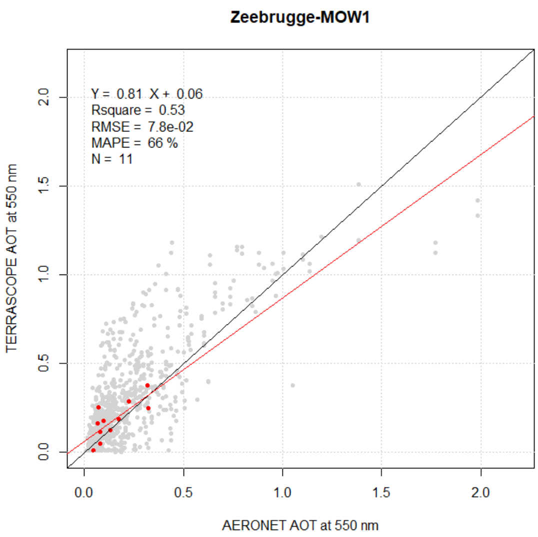


Figure 6.12 Scatterplots of AOT at 550 nm used in the Terrascope chain compared to AERONET measurements for individual sites. The red dots represent the values for each specific site, while the grey dots are all match-ups.

Based on these plots it becomes apparent that the current Terrascope chain is not equally suited for desert-like areas. Both Banizoumbou and Sede-Boker show bad correlations. Banizoumbou is a large city at the border of desert and vegetation in Niger, while Sede-Boker is located in the desert of Israel.

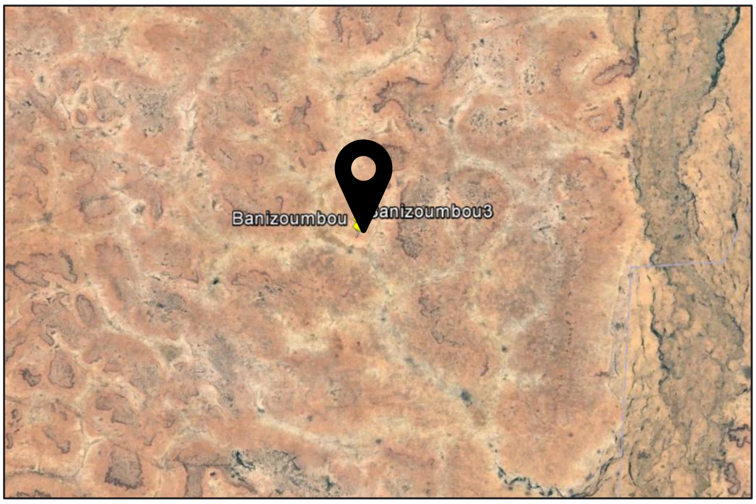


Figure 6.13: Location of Banizoumbou AERONET station in Niger. © Google Earth.

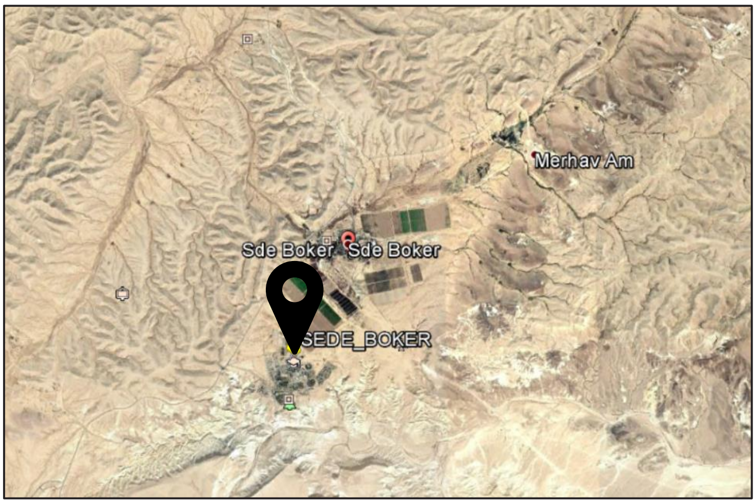


Figure 6.14 Location of the SEDE-BOKER AERONET station in Israel. © Google Earth

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ANNEX I – MODTRAN5 LUT input parameters

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

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

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

The breakpoint positions for the different input parameters of the LUT are listed in Table A.1.

Table A.1: Breakpoints MODTRAN5 LUT

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