

Algorithm Theoretical Basis Document

OLCI Terrestrial Chlorophyll Index (OTCI)

Title: ATBD for OTCI

Document Number: S3-L2-SD-03-C14-UoS-ATBD_OTCI

Issue: 2

Revision: 0

Date: 29/04/2010

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|  UNIVERSITY OF Southampton | SENTINEL-3 L2 PRODUCTS AND ALGORITHM DEFINITION | Document Ref: S3-L2-SD-03-C14- UoS-ATBD_OTCI Issue: 2 Date: 29-04-2010 |
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Signature Table

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Document Change Record

| Version | Date | Author | Description |
|---------|------------|---------------------------------|--|
| 1.0 | 01/12/2008 | Jadu Dash | PDR release (initial version) |
| 1.1 | 01/11/2009 | Jadu Dash | PDR RID update |
| 2.0 | 27/04/2010 | Jadu Dash Francesco Vuolo | CDR: Effect of soil on OTCI is added , Information about flags and their definition is updated |

From version 1.1 To version 2

| Page | Section | Comments |
|-------|---------|--|
| 11 | 3.2 | Band numbers in the OTCI algorithm were changed to reflect the final OLCI bands |
| 14-15 | 3.5 | Effect of soil on OTCI is modified to incorporate filed data used for the analysis. |
| 18-19 | 3.9 | This section is modified to include updated information on quality flag definitions, However at this stage we have not done a proper investigation on the thresholds and condition to be used with these quality flags. Once we have more information on these issues we will update this section. |
| 21-22 | 5 | References were updated related to the changes in the text |

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1 INTRODUCTION

1.1 Acronyms and Abbreviations

| | |
|-------|--|
| ATBD | Algorithm Theoretical Basis Document |
| BOA | Bottom of Atmosphere |
| BRDF | Bidirectional Reflectance Function |
| FOV | Field-of-View |
| GMES | Global Monitoring for Environment and Security |
| LAD | Leaf Angle Distribution |
| LAI | Leaf Area Index |
| MERIS | Medium Resolution Imaging Spectrometer |
| MTCI | MERIS Terrestrial Chlorophyll Index |
| NDVI | Normalised Difference Vegetation Index |
| NIR | Near Infrared |
| OLCI | Ocean and Land Colour Instrument |
| OTCI | OLCI Terrestrial Chlorophyll Index |
| TOA | Top of Atmosphere |

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1.2 Purpose and Scope

This Algorithmic Theoretical Basis Document (ATBD) describes the algorithm used to estimate chlorophyll content over land from Level-1 OLCI products from the Sentinel 3 mission. The algorithm called the OLCI Terrestrial Chlorophyll Index (OTCI) is a unique chlorophyll index for OLCI data. This document identifies the source of input data; outlines the physical principles and mathematical background; justifies this algorithm and then explores its limitations and assumptions.

1.3 Algorithm Identification

The OLCI Terrestrial Chlorophyll Index (OTCI) will be produced globally at 300m spatial resolution for land from OLCI data on the Sentinel 3 mission. This will be a continuation of the MERIS Terrestrial Chlorophyll Index derived from MERIS data. Therefore, at the time of launch of Sentinel 3 there will be nearly 11 years of MTCI data (2002-2012). This data set could be used to monitor vegetation condition and health.

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2 ALGORITHM OVERVIEW

2.1 Objectives

Chlorophyll content plays an important role in determining the physiological status of a plant which is related to photosynthetic rate and varies temporarily and spatially. If we can estimate chlorophyll content in time and space, then we have a key input to models of terrestrial productivity, gas exchange and vegetation health. Several methods can be used to estimate the chlorophyll content of leaves (Datt, 1998; Gitelson and Merzlyak, 1998; Mariotti et al., 1996) and canopies (Daughtry et al., 2000; O'Neill et al., 2002; Peterson et al., 1988, Coops et al., 2003) via remote sensing. Such studies indicate that measures of reflectance in narrow red and near infrared (NIR) wavebands are required for accurate estimation and such data have recently been available from space. The Envisat MERIS Terrestrial Chlorophyll Index (MTCI) is designed to monitor vegetation condition via an estimation of chlorophyll content using reflectance in the red edge region of the reflectance spectra. Unlike conventional vegetation indices which are based on the normalised difference between reflected solar radiation in red and near-infrared wavebands, MTCI makes use of the shift of the 'red edge' where absorption drops dramatically as wavelength increases. The use of red shift means that the MTCI product remains responsive to even at the high chlorophyll content levels where conventional vegetation indices saturate. For instance, a recent study has demonstrated a significant doubling of the signal to noise ratio for MTCI compared to commonly used Normalised Difference Vegetation Index (NDVI) over areas of wooded landcover. Sentinel-3 spacecraft will carry a set of optical and microwave instruments, one of which is the Ocean and Land Colour Instrument (OLCI) having similar band configuration to MERIS. This will be a continuity of MERIS and therefore, there is a possibility of developing a chlorophyll index similar to MTCI. The proposed OTCI will be developed as a chlorophyll index for the OLCI data.

3 ALGORITHM DESCRIPTION

3.1 Theoretical Description

The spectral reflectance of vegetation is characterized by absorption features that are the result of electron transitions and vibrational stretching of organic and inorganic bonds. The main chemical constituent of leaves include chlorophyll, water, nitrogen and carbon containing compounds, comprising primarily protein, lignin and cellulose. Out of these chlorophyll is associated with the process of photosynthesis and together with water, temperature, nutrient availability, CO₂ and sunlight; determines the rate of primary productivity. Therefore, chlorophyll is an important driver for the whole ecosystem (Munden et al. 1994). When incoming radiation interacts with vegetation, some part of it is reflected, some absorbed and rest is transmitted. A typical reflectance spectrum of a vegetation canopy can be subdivided into 3 parts, visible (400- 700 nm), near-infrared (NIR) (701 – 1300 nm) and middle-infrared (1301- 2500 nm).

Chlorophyll is the major absorber of radiation in the visible region. Chlorophylls are of two types, chlorophyll-a and chlorophyll-b; chlorophyll-a content is usually two to three times that of chlorophyll-b and dominates absorption in 600-700 nm wavelengths (Lichtenthaler 1987). Other leaf pigments also have an important effect on the visible spectrum. For example, the yellow to orange-red pigment, carotene, has a strong absorption in the 350 - 500 nm range and is responsible for the colour of some flowers and fruits as well as leaves without chlorophyll. The red and blue pigment, xanthophyll, has strong absorption in the 350-500 nm range and is responsible for the leaf colour in autumn.

In the near-infrared spectral domain (701-1300 nm), leaf structure explains the optical properties. Near-infrared spectral region can be divided into two major spectral sub-regions: first, between 701 and 1100 nm, where reflectance is high, except in two minor water-related absorption bands (960 and 1100 nm) and second, between 1100 and 1300 nm, which corresponds to the transition between high near-infrared reflectance and water-related

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absorption bands of the middle infrared. The intensity of NIR reflectance is commonly greater than from most inorganic materials, so vegetation appears bright in NIR wavelengths.

The middle-infrared region contains information about the absorption of radiation by water, cellulose and lignin etc. Other biochemicals, which contribute to absorption in middle infra-red wavelengths, are starches, sugars, lipids and minerals. Curran (1989) presented a list of forty-four absorption features in the visible and near-infrared wavelengths which were related to foliar biochemical constituents.

The red edge is a region within the red-NIR transition zone of a vegetation reflectance spectrum and marks the boundary between absorption due to chlorophyll in the red region and scattering due to leaf internal structure in the NIR region (Horler et al. 1983). The red edge position (REP) can be defined as the maximum of the first derivative of the reflectance spectra of a leaf (Horler et al. 1983; Curran et al. 1990). Most commonly used techniques to estimate REP include (i) higher order curve fitting techniques (Demetriades-Shah 1990); (ii) an inverted Gaussian technique (Bonham- Carter 1988; Miller et al. 1990); (iii) a linear interpolation technique (Guyot et al. 1988, Danson and Plummer 1995) and (iv) a Lagrangian interpolation technique (Dawson and Curran 1998). However, REP techniques have some drawbacks and therefore could not be applied to operational global products, which includes saturation at high chlorophyll content and difficulties in applying spectrally discontinuous data. Therefore, the MERIS Terrestrial Chlorophyll Index was developed as a surrogate estimator of the REP and applied successfully to MERIS data. MTCI is now available as a standard L2 product from MERIS data.

3.2 Mathematical description of the algorithm

Spectral resolution of Sentinel-3 OLCI sensor in the visible and NIR region is similar to that of MERIS (figure 1). Therefore, the OLCI Terrestrial Chlorophyll Index (OTCI) will be similar to MTCI. This could be defined as:

$$OTCI = \frac{R_{band12} - R_{band11}}{R_{band11} - R_{band10}}$$

Where R_{band12} , R_{band11} , R_{band10} are the reflectance in band centred at 753, 709 and 681 nm of the OLCI sensor.

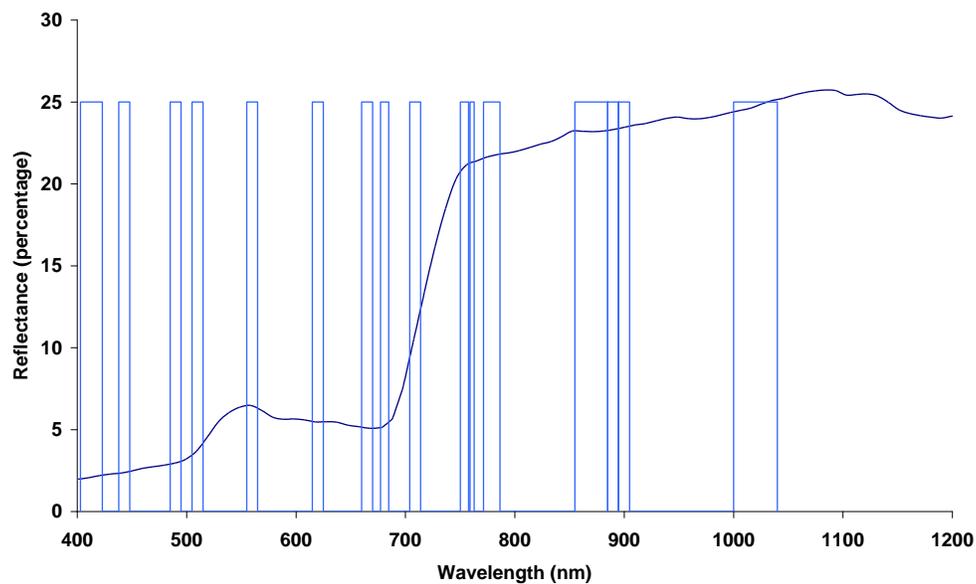


Figure 1. OLCI bands overlain on a vegetation spectral in the visible and NIR region.

OTCI was originally designed for top of canopy reflectance, but its adaptation to Rayleigh corrected in the MERIS processing chain has proven to be fairly robust to aerosol content. The baseline is thus to take Rayleigh corrected reflectance as an input. Three possible features: barren land, partial snow and low cloud cover could be a source of ambiguity in the OTCI estimation. Therefore, prior to the calculation of OTCI pixels covering these features should be removed. Detail parameters to identify these in the input data is under investigation. In addition to this the effect of view angle could have an effect on the OTCI estimation, particularly at higher view angle. Some results were presented in the next section from preliminary evaluation.

3.3 Indirect evaluation

A combination of LIBERTY (Leaf Incorporating Biochemistry Exhibiting Reflectance and Transmittance Yield (Dawson et al., 1998)) and the semi-discrete model (Gobron et al., 1997) was used to generate canopy reflectance spectra (400-2500 nm, spectral resolution of 5 nm) for a wide range of canopy (table 1) and non-canopy variables (table 2). The semi-discrete model was used because it has an advantage of describing vegetation canopy properties as a function of variable which can be physically measured, i.e. the number and orientation of the leaves within a canopy; the height of the canopy; soil albedo and the spectral reflectance and transmittance at leaf level. In addition, the semi-discrete model can generate reflectance data for various view and zenith angle relatively quickly than other canopy models with known canopy parameters.

Model data were averaged according to the band centre and band width of the OLCI standard bands to obtain the reflectance data, used to calculate OTCI.

| variables | Values |
|---|---------------------------|
| Chlorophyll content (mg m ⁻²) | 10-400 with 10 increments |
| Average internal cell diameter (µm) | 30 |
| Intercellular airspace determinant (unitless) | 0.005 |
| Leaf thickness (unitless) | 3 |
| Base line absorption (unitless) | 0.0004 |
| Albino leaf absorption (unitless) | 2 |
| Leaf water content (g m ⁻²) | 100 |
| Lignin or cellulose content (g m ⁻²) | 30 |
| Nitrogen content (g m ⁻²) | 1 |
| Leaf Area Index (unit less) | 1 -5 with increment of 1 |
| Leaf Angle Distribution (unitless) (using Bunnik's function) | 1 |
| Height of canopy (m) | 2 |
| Number of leaves per unit volume | 3184 |

Table 1. Leaf and canopy variables used to simulate data for the evaluation of OTCI.

| Variables | Values |
|-------------------------|-------------------------------|
| Sensor view angle(°) | -80 to +80 with 10 increments |
| Sun zenith angle (°) | 0 to 40 with 10 increments |
| Sun azimuth angle(°) | 0,180 |
| Soil type (Price, 1995) | 2, 3,4,5,6 |

Table 2. Non leaf and canopy variables used to simulate data for the evaluation of OTCI.

3.4 Relationship between Chlorophyll content and OTCI:

Figure 2 shows the relationship between chlorophyll content and OTCI derived from model data for 20 degree Sun Zenith angle and nadir view. It suggested that there was a strong linear relationship between OTCI and chlorophyll content with coefficient of determination R^2 nearly equal to 1. There was a slight deviation at very low chlorophyll content.

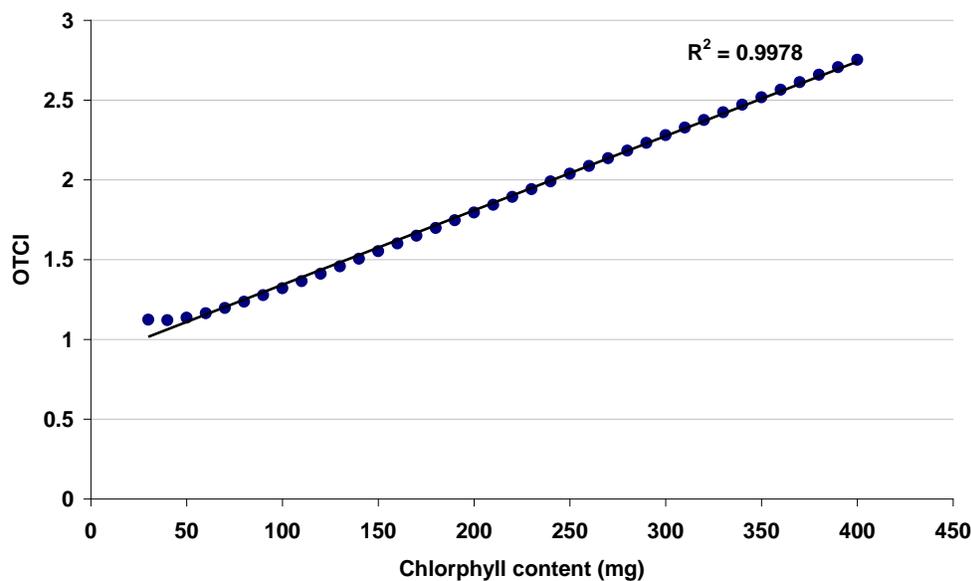


Figure 2: Relationship between OTCI and chlorophyll content.

3.5 Effect of Soil type:

The variation in the OTCI due to soil water content, changes due to different soil type (structure and chemistry) and the effect of the soil at low vegetation cover using data from field and satellite data were investigated.

For a given location, such as a field, soil mineral components and organic matter as well as soil structure should reveal only small modifications within the course of a vegetation period. Instead, surface water content might change depending on weather conditions and soil water storage capacity (Weidong et al., 2002). Richter et al. (2008, 2009) carried out an analysis to quantify the relationship between the soil reflectance and the soil surface water content (θ).

Data from this spectral measurement experiment were used to evaluate the effect of changing soil water content on the OTCI. Results indicated that for a given soil type in undisturbed conditions, OTCI variability is very limited and soil water content affected only minimally the chlorophyll index. In particular, the OTCI varied between 1.19 and 1.31 with a standard deviation of 0.05.

| Soil surface water content | OTCI |
|----------------------------|-------|
| 0% | 1.31 |
| 0.74% | 1.23 |
| 1.68% | 1.19 |
| 5.03% | 1.22 |
| 26.69% | 1.28 |
| Mean | 1.244 |
| St.Dev. | 0.050 |

Table 3 MTCI variability for the soil water content experiment

A second data set of 19 field spectral measurements of bare soils, acquired in the framework of the project ‘Participatory multi-Level EO-assisted tools for Irrigation water management and Agricultural Decision-Support’ (PLEIADeS) (D’Urso et al., 2009), was considered to test the OTCI. Results confirmed that in bare soil conditions OTCI presents a very low variability (min= 1.4; max= 1.8; mean=1.66; st.dev.=0.21) demonstrating the robustness of the chlorophyll index at different soil water content levels and for a limited variability of soil type.

Under different soil conditions, with similar vegetation cover, OTCI values were comparable relatively to the spectral reflectance data used. Different data sets from field experiments were exploited to demonstrate the robustness of the OTCI. Soil water content and soil type (structure and chemistry) did not reveal significant effects on the OTCI.

3.6 Effect of view angle:

Effect of view angle on the OTCI values were investigated for a range of view angles from -80° to +80° with 2° increment and for a range of chlorophyll concentration and LAI. This was combined with range of soil type. It was observed that the effect of view angle is quite

significant at low LAI and chlorophyll concentration. However, this effect was minimal for high LAI and chlorophyll concentration. In most cases the variation within -30° to $+30^\circ$ was not significant as compared to the OTCI values at nadir. In general there is an increase in the OTCI values with increase in view angle. And in most cases it was systematic. Therefore, it may be possible to determine this systematic increase in OTCI values and a correction factor may be used. Further investigation is underway to quantify the systematic increase.

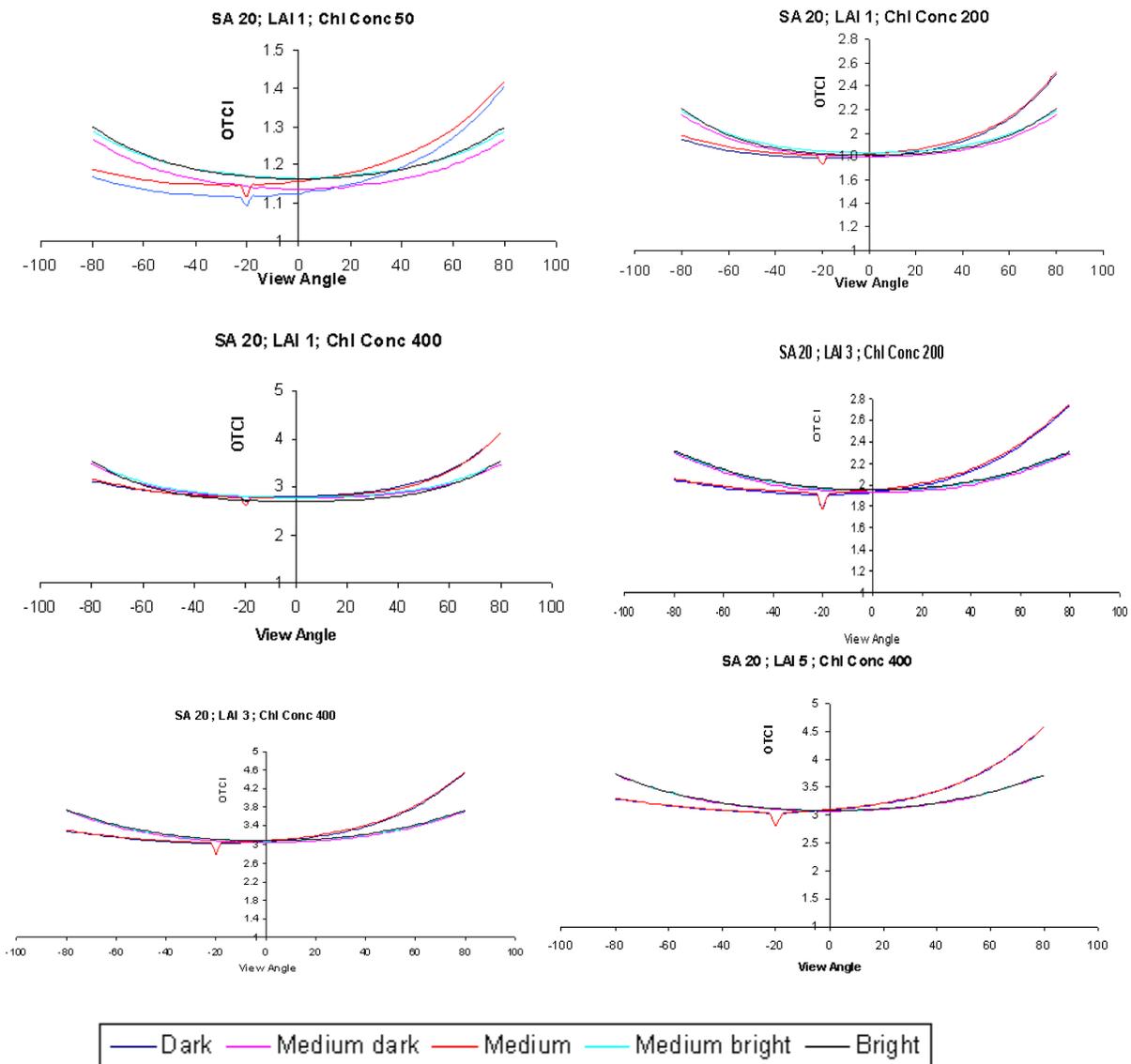


Figure 3. Effect of view angle on the OTCI.

3.7 Practical consideration

3.8 Processing method

In order to avoid meaningless values and numerical problems, input spectra shall be screened first for clouds, water and non-vegetated land surfaces. It then includes some simple spectral tests; one of which uses an additional reflectance at a second NIR band. Based on the processing, the expected accuracy of the product will be estimated. OTCI was originally designed for top of canopy reflectance, but its adaptation to Rayleigh corrected data in the MERIS processing chain has proven to be fairly robust to aerosol content. The baseline is thus to take Rayleigh corrected reflectance as an input.

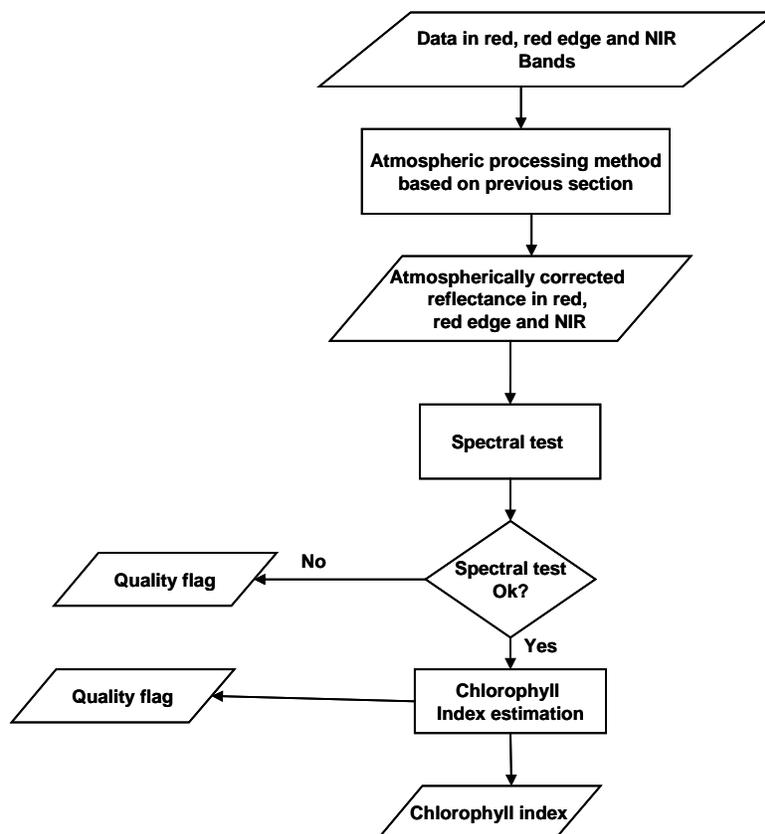


Figure 4. Outline of the chlorophyll index algorithm for OTCI.

3.9 Quality control and diagnostics

Quality control is essential to produce robust and reliable biophysical products from satellite data. Two major factors affect the quality of retrieval of biophysical variables: (i) problems with input data (for example, L1b) and (ii) conditions with satellite observations which make the retrieval of biophysical variables unreliable (for example, atmospheric condition, high sun sensor angles etc). Some of these factors may be generic and may affect most of the biophysical variable retrieval, whereas some factor may be specific to particular biophysical variables. In the current processing OTCI relies on the Rayleigh correction of normalised surface reflectance in bands 10, 11 and 12 and processing algorithm performance check over difference in reflectance in these bands. To make the index robust and to provide uncertainty due to non canopy variables the following flags should be used.

Input data quality flag: This will check the quality of the three input bands (band 10, 11 and 12). In addition the difference between band 10 and 11 and difference between band 11 and 12, to see if the difference is too low or negative etc. for the pixel to be classified as vegetation. Threshold will also be set for identifying bare soil conditions.

Aerosol related flag: Based on the initial evaluation we would like to use a flag for high Aerosol content. However, it was found that the DDV algorithm used in the current L2 processing of MERIS was not appropriate for aerosol retrieval in some cases, so we would like to have the flag based on BEAR or an advanced algorithm. ***Since there are no aerosol products from OLCI Land processing, we would like to use the Aerosol from the synergy product. This will provide better confidence on the OTCI product, particularly at high aerosol content. However, this will be an evolution as the baseline is that the processors aren't dependant on each other.***

View geometry related flag: This flag will be applied for a higher view angle. We still need to define a threshold for this. However, initial investigation suggested that OTCI is relatively stable up to view angle of ± 30 degree.

Cloud and snow flag: We would like to have a flag for cloud shadow/ low lying cloud and partial snow cover. The cloud detection flag used in the current L2 processing does not account for this. However, the effect of could shadow and partial snow cover on OTCI is still under investigation. In addition we are not sure if the current or future L2 processing will have the ability to detect the cloud shadow/ partial snow cover. This needs further investigation.

Table below provides summary of the flags to be used with MTCI:

| Flag | Condition | Comment |
|----------------------|--|---|
| Input data quality | L2 B12, B11, B10 are Valid AND (B12-B11)>Threshold 1 AND(B11-B10)>Theshold2 | Currently in the DPM the exceptional handling uses nir3 and red and nir1 and red. We will further investigate the range and band to be used. Thresholds will be provided. |
| Aerosol related flag | Input data quality flag OK AND AOT > Threshold | Threshold needs to be defined. Also need to agree on which algorithm should be used to estimate AOT and its implementation in L2. |
| View angle flag | Input data quality flag OK AND view angle> Threshold AND Sun angle > Threshold | Initial investigation suggests OTCI is relatively stable up to view angle of ± 30 degree. We are thinking of a correction factor rather than flag here for higher view angles, based on an empirical relationship. This will only be applied if all other flags are OK. |
| Cloud and snow flag | Input data quality flag OK Cloud shadow and partial snow detected | This is under further investigation |

Table 4: Flag Criteria for OTCI

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The following conditions describe error or exception conditions, which can be flagged by setting the corresponding bit to 1. These are from preliminary investigation further conditions will be added later.

1. The land flag should be set to 1 if any pixel was not a land pixel.
2. The saturation flag should be set to 1 if any of the 3 spectral bands (band 10, 11 and 12) used by this algorithm were saturated.
3. The band flag should be set to 1 if data in one or more spectral bands was missing.
4. The overflow flag should be set to 1 if numerical overflow occurred while processing the data.

4 ASSUMPTIONS AND LIMITATIONS

The following assumptions were made in the design of the OTCI algorithm.

1. All water pixels masked prior to estimation of OTCI.
2. Non-saturated MERIS level 2 normalised surface reflectances available in band 10, 11 and 12.
3. Positive Level 2 normalised surface reflectances available in band 10, 11 and 12.
4. Level 2 normalised surface reflectances used as input corrected for the seasonally variable distance between the Earth and Sun.
5. Adjacency effects ignored.
6. Substantial atmospheric aerosol loads, as observed in dust storms and heavily polluted area screened out or their occurrence was infrequent.

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