SeaShark SeaWiFS Level 2 Processing

Guide to Products

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Summary: This document describes algorithms employed by SeaShark to generate Level 2 SeaWiFS products. It guides interpretation of these products by a User, and highlights processing options available.

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1 INTRODUCTION

1.1 Purpose

The purpose of this document is to describe the scientific algorithms used in the SeaShark processing suite for the generation of SeaWiFS Level 2 ocean colour products. It provides the source of the algorithms, the mathematical form, the units and approximate dynamic range of the output (when unscaled from the integer representation in the output files, and where appropriate), indicates the algorithmic validity, and provides a guide in interpretation of the products.

1.2 Scope

SeaShark is software that provides a capability for the processing, archiving and dissemination of data from the SeaStar OrbView-2 (SeaWiFS) and NOAA Polar Orbiter satellites. This document describes algorithms for the processing to Level 2 of SeaWiFS data. Certain topics are not discussed here.

- Scientific validity of the algorithms. These have been tested by scientists and the results published, but the state of the art is continually progressing as data is produced by satellites and corresponding ground truth measurements are made.
- Acquisition and suitability of ancillary data (required for correcting measurements for the effects of the atmosphere). This is documented in the Software User Manual [10].

This document is designed to be useful for the following purposes:

- to indicate the form of the algorithms underlying the SeaWiFS level 2 products;
- to support interpretation and indicate validity of the products;
- to indicated which combinations of bands are relevant for particular applications.

It applies to SeaWiFS Level 2 products in CEOS format [8] and the chlorophyll *a* FDP [7].

1.3 Document Structure

The document consists of this introduction, a summary of the products available, and the algorithmic descriptions. The latter are subdivided according to the approximate stage in the processing chain that the algorithms are used.

1.4 Definitions, Acronyms and Abbreviations

This section lists the definitions of all terms, acronyms and abbreviations, or refers to other documents where the definitions may be found.

Term	Definition
AVHRR	Advanced Very High Resolution Radiometer
CEOS	Committee on Earth Observation Satellites
CZCS	Coastal Zone Colour Scanner
DCW	Digital Chart of the World
ESA	European Space Agency

Table 1 Definitions, acronyms and abbreviations

Term	Definition
ESRIN	European Space Research INstitute
FDP	Fast Delivery Product
GAC	Global Area Coverage
HRPT	High Resolution Picture Transmission
LAC	Local Area Coverage
NASA	National Aeronautics and Space Administration
NOAA	National Oceanic and Atmospheric Administration
ODOC/ODOCA	Optically Dissolved Organic Carbon
OSC	Orbital Sciences Corporation
PAR	Photosynthetically Absorbed Radiation
PML	Plymouth Marine Laboratory
SeaDAS	SeaWiFS Data Analysis System
SeaWiFS	Sea-Viewing Wide Field-of-View Sensor
SHARK	Station HRPT Archiving and Reprocessing Kernel
SPM	Suspended Particulate Matter

Table 1 Definitions, acronyms and abbreviations

1.5 References

[1] SeaWiFS Algorithms, Part 1, C. R. McClain *et al.*, SeaWiFS Technical Report Series, NASA Technical Memorandum 104566, Vol. 28, June 1995.

[2] The SeaWiFS CZCS-Type Pigment Algorithm, Aiken *et al.*, SeaWiFS Technical Report Series, NASA Technical Memorandum 104566, Vol. 29, June 1995.

[3] G. F. Moore, J. Aiken, S. J. Lavender and H. Botrell, “The atmospheric correction of water colour and the quantitative retrieval of biogeochemical variables in case 2 waters: application to MERIS”, submitted to Int. J. Rem. Sens., 1996.

[4] H. R. Gordon, H. R. and M. Wang, “Retrieval of water-leaving radiance and aerosol optical thickness over the oceans with SeaWiFS: a preliminary algorithm”, Appl. Opt., 33(3), 443-453, 1994.

[5] W. W. Gregg and K. L. Carder, “A simple spectral solar irradiance model for cloudless maritime atmospheres”, Limnol. Oceanogr., 35(8), 1657-1675, 1990.

[6] Case Studies for SeaWiFS Calibration and Validation, Part 1. McClain *et al.*, SeaWiFS Technical Report Series, NASA Technical Memorandum 104566, Vol. 13, January 1994.

[7] FDP Generic Format, SHK.ICD.003, Issue 1.0, 27 November 1996.

[8] Instrument Data Product Format – SeaWiFS Flexible Format, SHK.ICD.004, Issue 1.0, 28 October 1997.

[9] SeaShark SeaWiFS Level 2 Processing Architectural Design Document, SHK.ADD.002, Issue 1.0, 23 July 1997.

[10] SeaShark Software User Manual Version 3.0, SHK-SUM-3.0, Issue 1.0, 16 December 1997.

[11] Case Studies for SeaWiFS Calibration and Validation, Part 4. E.-n. Yeh *et al.*, SeaWiFS Technical Report Series, NASA Technical Memorandum 104566, Vol. 41, August 1997.

[12] The Simulated SeaWiFS Data Set, Version 1. W. Gregg *et al.*, SeaWiFS Technical Report Series, NASA Technical Memorandum 104566, Vol. 9, May 1993.

2 SUMMARY OF SEAWIFS LEVEL 2 PRODUCTS

A summary of the level 2 products generated in SeaShark from SeaWiFS data is shown below. The format of the products is given in references [7] for the FDP and [8] for the standard CEOS product. For level 2 processing, ancillary data is required; grids of the data values used are contained in the Annotation file of the CEOS product.

2.1 Product Bands Generated

Product	Description or Note
Normalised water leaving radiances at SeaWiFS bands 1–5, $L_{WN}(\lambda)$	Produced by the atmospheric correction.
Aerosol radiances at SeaWiFS bands 6–8, $L_a(\lambda)$	Produced by atmospheric correction, these are the calculated radiances due to the effects of aerosol in the atmosphere.
CZCS-type pigment	Amount of pigment in the water measured using a method derived from that used in processing CZCS data.
Chlorophyll *a*	Amount of chlorophyll type *a* in the water.
Suspended particulate matter (SPM)	Amount of sediment in the water. Silt, mud or coccolith in origin. Sedimented water is always case II by definition.
Coccolithophore	Amount of sediment in the water if determined to be coccolith in origin.
Carotenoid	Amount if carotenoid pigment in water
ODOC	Amount of ODOC in water (dissolved organic carbon)
Normalised diffuse attenuation coefficient for downwelling irradiance, K_d'	Coefficient of water clearness
PAR	Radiation available for photosynthesis
Aerosol optical thickness at 865 nm (τ_a)	Coefficient of the atmospheric clearness excluding the effects of scattering from air molecules and the absorption of ozone.
Correction epsilon ε	Characterisation of the type of aerosol
Flags	
Atmospheric correction failure	Set if correction algorithm is unsuccessful. (Fatal)
Land	Determined through navigation. (Fatal)
Missing ancillary data	Set if some ancillary data is not available.
Sun glint	Warning that sunlight may be reflected into sensor.
Bright pixel	Pixel is too bright. (Fatal)
Stray light	Warning that nearby pixel is bright.
Large spacecraft zenith angle	Warning of unfavourable satellite geometry.
Large solar zenith angle	Warning of unfavourable solar geometry.
Low water leaving radiance	Correction has produced unexpectedly low result.
Zero water leaving radiance	Correction has produced unphysical result.
Cloud/ice	Cloud or ice detected. (Fatal).
Case II water	Water is Case II sediment or Gelbstoff.
Case IIy water	Water is not sediment but Gelbstoff.
High aerosol concentration	Probably too much aerosol for accurate correction.
Colour composite	Top of atmosphere colour composite

Table 2 CEOS SeaWiFS level 2 product summary

Most algorithms have coefficients that may be configured within SeaShark, usually from the atmospheric correction (Level2/SeaWiFS_atmospheric_correction.cfg) or geophysical product (Level2/SeaWiFS_geophys.cfg) configuration files. Instructions for performing this are contained in the Software User Manual [10]. The coefficients are recorded within CEOS products [8].

Flags marked ‘fatal’ in Table 2 are indicated within the FDP, but warning flags are disregarded [7].

2.2 Product Validity

	Atmo. corr’n fail **Land** **Bright pixel** **Cloud/ice**	**Low w.l. radiance** **Zero w.l. radiance** **High optical thickness** **Large zenith angle** **Missing ancillary data**	**Sun glint** **Stray light**	**Case I**	**Case IIs**	**Case IIy**
Radiances	TOA	**?**	**?**			
CZCS pigment	✗	**?**	**?**			
Chlorophyll *a*	✗	**?**	**?**			
SPM	✗	**?**	**?**	✗		**?**
Coccolithophore	✗	**?**	**?**	✗		**?**
Carotenoid	✗	**?**	**?**		✗	✗
ODOC	✗	**?**	**?**			
K_d	✗	**?**	**?**			
PAR	✗	**?**	**?**			
τ_a	✗	**?**	**?**			
ε	✗	**?**	**?**			
Colour composite			**?**			

Table 3 Impact of flag conditions on product validity

The impact of level 2 flag conditions on product validity is shown in Table 3. Key: ✗ – failure (set to zero); **?** – warning (product unreliable); TOA – substituted by top-of-atmosphere radiances.

3 DETAILED ALGORITHMIC DESCRIPTION

This section discusses the individual algorithms employed within the level 2 processing modules of SeaShark. These are subdivided into the following sections corresponding to the processing stage where each algorithm is employed:

- Pre-correction flagging algorithms,
- Atmospheric correction algorithms,
- Post-correction flagging algorithms, and
- Geophysical product algorithms.

Also included are descriptions of flags that are not calculated via imagery based algorithms such as land and missing ancillary data. Note that no flags are fatal as far as the colour composite product is concerned.

The structure of the descriptions is as follows: a discussion and the mathematical form (where appropriate) of the algorithm is given, followed by a list of (a) the source of the algorithm, (b) the validity, (c) the units where appropriate, (d) for flags only, the meaning or interpretation of the flag condition and (e) for products only, the approximate range of the result.

It should be noted that the potential range of an algorithm may be constrained by SeaShark's scaling parameters because of the scarcity of very high or very low values. The range is also primarily applicable to ground-based measurements where area under consideration is orders of magnitude smaller than the best satellite resolution. This has the effect of smoothing out high concentrations occurring over sub-pixel sized areas. Scaling factors and thresholds are read from SeaShark's order processing configuration file (order.cfg), and recorded in the CEOS leader file, Satellite Information Record, and FDP text file.

3.1 Pre-correction flagging algorithms

There are four flagging algorithms required to select data suitable for further processing within the chain, and before the atmospheric correction takes place: the identification of cloud, stray light, sun glint and land. If the cloud flag is set, no further processing on the associated pixel is performed, since the algorithms are inapplicable. If the stray light condition is met, or if the pixels are identified as being in sun glint, the associated flags are set as warnings that the processing may be unreliable. (The stray light condition occurs around bright pixels: the instrument has a finite recovery time to a bright target, thus flags are set in surrounding pixels to warn that results may not be accurate. The bright pixel condition normally occurs when any of the recorded radiances values exceed the knee value of the instrument's bi-linear gain.)

Details of the four algorithms are given in the following subsections.

3.1.1 Cloud algorithm

The cloud flagging algorithm is given as follows. Pixels having an 865 nm albedo (α) greater than 0.9% are flagged as cloud or ice. This may be re-expressed as pixels having a 865 nm radiance greater than a threshold value ($I_{threshold}$) are flagged as cloud or ice through the following, where F_0 is the solar flux at 865 nm:

$$I_{threshold} = \frac{F_0 \alpha}{\pi}$$

The algorithm therefore compares the band 8 top of atmosphere radiance with the threshold value (as calculated for mean Earth-Sun distance) contained in the geophysical product configuration file, and sets the flag if the radiance is exceeded. Thresholds employed are recorded in the CEOS leader file, Thresholds and Correction Data Record.

Source: Volume 28 of the SeaWiFS Technical Report Series, [1]. Note, though, that there are inconsistencies in this source and the references it in turn cites. The implementation is therefore not identical.

Validity: All water types and over land. May be triggered by ice.

Units: None (flag)

Meaning: Fatal flag – no further processing occurs if this flag is set.

3.1.2 Stray light and bright target flags

The bright target condition consists of a simple threshold test, with configurable values. The stray light flag is set for pixels adjacent to any pixel masked for bright target in NASA's GAC configuration, therefore for LAC data, the surrounding pixels up to four away require masking.

The radius of surrounding pixels (expressed in terms of number of pixels perpendicular or parallel to the scan line) that are flagged is configurable. Coefficients are read from SeaShark's geophysical product configuration file, and recorded in the CEOS leader file, Thresholds and Correction Data Record.

For LAC data with the extent of bright pixel processing set to 4, the flagging is performed as indicated in the diagram below, where B represents a bright pixel, O represents a 'normal' pixel, and X a stray-light-flagged pixel:

```
OOOOOOOOO               OOOOXOOOO
OOOOOOOOO               OOOXXXOOO
OOOOOOOOO               OOXXXXXXO
OOOOOOOOO               OXXXXXXXO
OOOOBOOOO processed->   XXXXXXXXX
OOOOOOOOO               OXXXXXXXO
OOOOOOOOO               OOXXXXXXO
OOOOOOOOO               OOOXXXOOO
OOOOOOOOO               OOOOXOOOO
```

The centre pixel is flagged as both stray light and as a bright target.

Source: Volume 28 of the SeaWiFS Technical Report Series, [1]

Validity: All water types, and over land

Units: None (flag)

Meaning: Bright target—fatal flag.
Stray light—warning, pixels may be contaminated by sensor "ringing" caused by the bright target so results should be treated with caution. No effect in FDP.

3.1.3 Sun glint

The probability of a pixel being contaminated by glitter is a function of sea surface wind speed, W, and satellite viewing geometry, namely the solar azimuth and zenith angles (Φ_0 and θ_0 respectively) and the satellite azimuth and zenith angles (Φ and θ respectively). A probability parameter P_σ is defined by:

$$P_\sigma = \frac{1}{\pi\sigma^2}\exp\left(\frac{-\tan^2\theta_n}{\sigma^2}\right)$$

where σ^2 is the mean square surface slope distribution which increases linearly with wind speed:

$$\sigma^2 = 0.003 + 0.00512W$$

The zenith angle θ_n of the vector normal to the surface vector for which glint will be observed will be derived from the surface reflection angle ω:

$$\theta_n = \cos^{-1}\left(\frac{\cos\theta + \cos\theta_0}{2\cos\omega}\right)$$

where:

$$\cos 2\omega = \cos\theta\cos\theta_0 + \sin\theta\sin\theta_0\cos(\Phi - \Phi_0)$$

A pixel will be flagged as sun glint contaminated if the calculated value of P_σ is greater than or equal to a given threshold value, which is contained in the geophysical configuration file. For a known viewing geometry the sea surface wind speed and the assigned threshold value can be determined. The number of pixels flagged decreases as the threshold value increases, and increases with wind speed.

The wind speed value should be sourced from meteorological data, or, if not available, climatological data. The angles are sourced from the navigation information. The probability threshold is recorded in the CEOS leader file, Threshold and Auxiliary Data Record, and wind speed in the annotation file, Annotation Data Record, at navigation grid points.

Source: Case Studies for SeaWiFS Calibration and Validation, [6]

Validity: All water pixels

Units: None (flag)

Meaning: All results should be treated with caution.

3.1.4 Land flagging

There is no algorithm as such for land flagging, since it is derived from SeaShark's navigation. With land masking enabled, all pixels flagged as land by the DCW are not processed, and the Level 2 Land flag is set. If land masking is disabled, the Land flag remains unset and processing is attempted, however most or all pixels collected over land will not fit the atmospheric correction model, and will be flagged Atmospheric correction failure (fatal). Land masking is controlled by SeaShark's order processing configuration file, and recorded in the CEOS leader file, Thresholds and Correction Data Record.

Source: Internal navigation within SeaShark. If required through the configuration files (see [10] for details), land pixels are masked to inhibit further processing. N.B. Regardless of the state of the configuration files, land is always indicated within the CEOS annotation file, Annotation Data Record.

Validity: All pixels.

Units: None (flag).

Meaning: Fatal—no further processing is carried out if the flag is set.

3.2 Atmospheric correction algorithms

There are three elements to the atmospheric correction algorithms: Rayleigh correction (for the effects of molecular scattering, calculated from a database of results from SeaDAS v2.0), PML correction (for the effects of case II waters), and the Wang correction (for the effects of aerosol scattering, derived from the Gordon and Wang method [4]). The PML correction sits between the Rayleigh and Wang corrections, and acts as a pre-conditioner with two roles: to derive case II related parameters, and to prepare case II pixels for the Gordon and Wang correction.

3.2.1 Rayleigh correction

The Rayleigh correction applies to the effects of molecular scattering in the atmosphere. Because molecular scattering is a function of the amount of scatterer, it is therefore a function of the surface pressure. This varies fairly smoothly, thus the Rayleigh correction uses a built-in optimization that calculates the scattering typically every sixth pixel – the exact spacing depends on the number of pixels per scan line. One function is used to calculate the initial correction for the subsampled array; a second is used to perform the interpolation so that each pixel has associated Rayleigh corrected radiances.

The correction is based on a data file of pre-calculated results. This database has been constructed using a polarised radiative transfer code, therefore the results should be very accurate.

Source: The correction database is extracted from Gordon and Wang’s tabulation in SeaDAS v2.0[1] on the recommendation of PML.

Validity: All water pixels. (It is assumed that the surface is at sea level, so although the algorithm is scientifically valid over land, SeaShark does not apply it.)

Units: Not applicable.

3.2.2 PML correction

3.2.2.1 Overview

The PML correction sets the case II flag if appropriate, and calculates the SPM value. There are two potential case II conditions: sediment (denoted *s*) and Gelbstoff or yellow substance (denoted *y*). The case II flag is set for both of these conditions, and the case IIy algorithm

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[1] SeaDAS software may be freely downloaded from NASA (`http://shark.gsfc.nasa.gov`). Copyright is acknowledged.

(described later) determines the nature of the water, and sets the case IIy flag if Gelbstoff is detected, or leaves it false otherwise. The truth table is shown in Table 4.

Case II flag	Case IIy flag	Interpretation	Note
0	0	Case I water	Sediment and coccolithophore zero
0	1	Invalid state	Never occurs
1	0	Case IIs water	Sediment value, possibly coccolithophore
1	1	Case IIy water	Sediment and coccolithophore values are set, but are not trustworthy

Table 4 Case II / Case IIy flag truth table

The PML correction preprocesses the satellite data stream to establish the nature of the underlying water. This is done by deriving an Ångström-type exponent from the Rayleigh-corrected reflectances in bands 7 and 8, and using it to calculate a ‘predicted’ reflectance for band 6. If the difference between this and the actual Rayleigh-corrected reflectance exceeds a predetermined threshold (dependant upon the scene geometry, and obtained from a look-up table stored as a SeaShark configuration file), the underlying water is deemed to be case II. A bright pixel model is then used to compare the measured reflectances with tabulations (stored as SeaShark configuration files) of known reflectance and suspended particulate matter (SPM) levels across SeaWiFS bands 6 to 8, and the estimated SPM contribution to reflectance is determined. This effects of the latter may then be corrected, and the corresponding concentration output.

The Wang correction (see the next section) is subsequently used to perform the atmospheric correction, using either the unaltered case I reflectances, or the corrected case II reflectances.

3.2.2.2 Algorithms (including SPM generation)

The Ångström-type exponent, A, is given by

$$A = (\ln\varepsilon_j)/\left(\ln\left[\frac{765}{865}\right]\right) \quad \text{, where } \varepsilon_j = \frac{\rho_7}{\rho_8}$$

and ρ_n is the Rayleigh-corrected reflectance for channel n.

The predicted band 6 reflectance is calculated using

$\rho_{6,a} = \rho_8(670/865)^A$. The pixel is deemed to be case II if

$\rho_6 - \rho_{6,a} > \text{threshold}(\text{pixel geometry})$. The threshold is determined via a look-up table generated by PML.

For case I pixels, no further processing occurs within the PML atmospheric correction; the original reflectances are passed on to Wang for further processing. For case II pixels, the following process is applied.

$k_s = \frac{\bar{\rho}_7}{\bar{\rho}_8} - 1.0$, where the overbars denote averages: these values are constants.

The reflectance due to sediment is estimated using $\rho_{s,8} = \frac{\rho_8(\varepsilon_j - 1.0)}{k_s}$.

This value is used as a query into the band 8 sediment/reflectance look-up table to generate the corresponding estimated sedimentation level. Reflectance due to aerosol is estimated by subtracting the sediment reflectance from the Rayleigh corrected reflectance:

$$\rho_a = \rho_8 - \rho_s .$$

The estimated sediment contribution to reflectance is then refined by solving (using a modified Newton method) the simultaneous equations

$$0 = \rho_7 - \rho_a - T_7 \rho_{s,\,7}(S)$$

$$0 = \rho_8 - \rho_a - T_8 \rho_{s,\,8}(S)$$

where T is the diffuse transmittance, and ρ_a and S are the iterated variables.

When the iteration has converged, the sediment quantity may be extracted, and the sediment reflectance calculated by cross referencing the quantity with the associated tables for bands 6, 7, and 8.

For case II pixels, the Rayleigh-corrected and case II corrected reflectance for bands 6 to 8 (band represented by *i*) is given by

$$\rho_{\text{Rayleigh and case II corrected, } i} = \rho_{\text{Rayleigh corrected, } i} - \rho_{s,\,i} T_i .$$

Source: Plymouth Marine Laboratory [3]

Validity: Case II flag: all waters.
SPM: case IIs waters (i.e., waters not flagged as case IIy).

Units: SPM: g m^{-3}

Range: SPM: 0.1–1000.

3.2.3 Wang correction (including aerosol tau and epsilon)

The Wang correction applies to the effects of aerosol scattering in the atmosphere.

The Wang correction returns the water leaving radiance, the epsilon value, and the aerosol optical thickness at 865 nm.

The correction is based on a data file of pre-calculated results.

Source: The aerosol database files are extracted from Gordon and Wang’s tabulation in SeaDAS on the recommendation of PML.

Validity: All water pixels.

Units: Both aerosol optical thickness (tau) and epsilon are dimensionless.
Water leaving radiance is in mW cm^{-2} µm^{-1} sr^{-1}.

Range: Not known.

3.3 Post-correction flagging algorithms

The post correction flagging algorithms comprise the following:

- High optical thickness,
- Low water leaving radiance,
- Negative water-leaving radiance,

- Case 2 y (Gelbstoff flag),
- High solar zenith angle,
- High view zenith angle,
- Missing ancillary data.

3.3.1 High optical thickness

This is a simple threshold test. The flag is set if the optical thickness (tau) exceeds the value in the geophysical product configuration file (recorded in the CEOS leader file, Thresholds and Correction Data Record). Aerosol corrections are unreliable when the optical thickness is large.

Source: Volume 28 of the SeaWiFS Technical Report Series, [1]

Validity: All water types where successful atmospheric correction has taken place.

Units: None (flag)

Meaning: Warning flag that atmospheric correction is likely to be inaccurate and therefore all pixel results should be treated with caution.

3.3.2 Low water leaving radiance

This is a simple threshold test: the flag is set if the calculated normalised water-leaving radiance at 555 nm is below 0.21 mW cm^{-2} μm^{-1} sr^{-1}. This threshold is set by the geophysical product configuration file and recorded in the CEOS Threshold and Auxiliary Data Record. The value is based on 75% of the normal water-leaving radiance at 555 nm for pure sea water.

Source: Volume 28 of the SeaWiFS Technical Report Series, [1]

Validity: All water types.

Units: None (flag).

Meaning: Warning flag. Treat all results with caution.

3.3.3 Negative water leaving radiance

This is a simple threshold test. The flag is set if the calculated water-leaving or aerosol radiance for any of the channels is below 0.0 mW cm^{-2} μm^{-1} sr^{-1}.

Source: Volume 28 of the SeaWiFS Technical Report Series, [1]

Validity: All water types.

Units: None (flag).

Meaning: Warning flag. At least one water-leaving radiance was negative (through modelling error) and has been set to zero. Treat all results with extreme caution.

3.3.4 Case IIy (Gelbstoff) flag

For discussion of the case IIy flag, please refer to section 3.2.2.1. The case IIy algorithm is based on the following:

Calculate $H(2,5)$, $H(3,5)$ and $H(4,5)$, where

$$H(x, y) = \frac{(\rho_x/\rho_y) - A_1}{A_2 - A_3(\rho_x/\rho_y)}$$

, and x and y represent the SeaWiFS channels.

Set the flag if $H(2, 5) \geq B_1 H(3, 5) \geq B_2 H(4, 5)$.

The *A*'s and *B*'s are all set through SeaShark's geophysical configuration file and recorded in the CEOS leader file, Thresholds and Correction Data Record. The values are as follows.

$B_1 = B_2 = 1.2$

	A_1	A_2	A_3
H(2,5)	9.55	0.5157	10.31
H(3,5)	5.29	0.71944	4.23
H(4,5)	3.17	0.53573	2.16

Table 5 Case IIy algorithm coefficients

Source: PML: personal communication from Dr Gerald Moore to Roland Flowerdew.

Validity: All case II waters.

Units: None (flag).

Meaning: State flag. Most results continue to be valid—see Table 3 and individual algorithm descriptions for full details.

3.3.5 High solar and satellite zenith angles

These are simple threshold tests. The appropriate flags are set if the solar or satellite zenith angles (calculated from the image navigation) exceed 70°. These thresholds set by the geophysical product configuration file, and recorded in the CEOS leader file, Threshold and Auxiliary Data Record.

Source: Volume 28 of the SeaWiFS Technical Report Series, [1]

Validity: All pixels.

Units: None (flag).

Meaning: Warning, all data values should be treated with caution. Results may be unreliable due to unfavourable geometries.

3.3.6 Missing ancillary data

There is no algorithm as such for this flag.

Source: If, in the original ancillary data source (whether climatologic or meteorologic in origin) any of the data points are missing and have been filled by interpolation, the missing ancillary data flag is set.

Validity: All pixels.

Units: None (flag).

Meaning: Each request for ancillary data at a given location by the processing chain is handled by a data management program. Usually, the image pixel location will not match the ancillary data grid of values, nor will it usually match temporally. Most ancillary data values are constructed by interpolation from the surrounding four points spatially, and from two temporal data files, i.e., from eight points in total. There are four ancillary data types (surface pressure, column ozone, humidity and surface wind speed) thus each image pixel may depend on 32 grid points within the ancillary data sets. If any of these 32 points have been mathematically generated (because, for example, of missing data), the missing ancillary data flag will be set. If the source ancillary data is patchy, the flag will appear frequently within the image file.

3.4 Geophysical product algorithms

The geophysical product algorithms comprise the following: chlorophyll *a*, CZCS-type pigment, carotenoid, K_d, ODOC, PAR, coccolithophore and colour composite. The first three of these are band ratio algorithms which are identical in algebraic form.

3.4.1 Band ratio algorithms (chlorophyll, CZCS-type pigment, carotenoid)

The chlorophyll *a*, CZCS-type pigment and carotenoid algorithms provide measures of the amount of pigments within the water. Chlorophyll *a* is one of three types of chlorophyll, the CZCS-type pigment algorithm provides a measurement similar to that derived from CZCS imagery, so is useful for historical comparison, and the carotenoid algorithm gives an indication of pigments in the water that are carotenoid in origin.

The band ratio algorithms – chlorophyll *a*, CZCS-type pigment, carotenoid – are of the form

$$P = \frac{\dfrac{L_{WN}(490)}{L_{WN}(555)} + C_1}{C_2 + C_3\dfrac{L_{WN}(490)}{L_{WN}(555)}}$$

where P is the pigment concentration, L the normalised water-leaving radiances at the specified channels, and the C's are tuneable coefficients. For chlorophyll *a* and CZCS pigment only: if the value of P is below a specified configurable threshold (2.0 mg m^{-3}), then a correction is applied, the final value being given by P_{corr}.

$$P_{corr} = C_4 P\left[\frac{L_{WN}(443)}{L_{WN}(555)} + C_5\right]^{0.5}$$

These parameters are read from the geophysical product configuration file, and recorded in the CEOS leader file, Geophysical Parameter Record. The values of the coefficients C (as at date of document) are shown in Table 6.

Algorithm	1	2	3	4	5
Chlorophyll *a*	–5.29	0.719	–4.23	1.455	–0.279
CZCS pigment	–5.29	0.592	–3.48	1.280	–0.163
Carotenoid	–5.29	0.719	–4.23	n/a	n/a

Table 6 Values of band ratio coefficients

Source: The SeaWiFS CZCS-type pigment algorithm, [2].

Validity: Chlorophyll *a* and CZCS-type pigment—all waters. Carotenoid—case I waters.

Units: mg m^{-3}.

Range: 0.01 to 100.

3.4.2 K_d algorithm

K_d is a coefficient representing the clearness of the water. The following description of the K_d algorithm has been supplied by Dr Gerald Moore of the Plymouth Marine Laboratory, UK. In SeaShark, the output is K_d' of the description below.

The current K_d' algorithm [11] uses the $L_{WN}(443)/L_{WN}(555)$ ratio, where K_d' is $K_d(490)–K_w(490)$.

$$\ln[K_d'] = -2.30261 - 1.29966 \ln[L_{WN}(443)/L_{WN}(555)]$$

In situ observations have show the algorithm is accurate up to $K_d' \approx 0.3$; however in coastal waters $K_d(490)$ may reach values of 1 or more. Under these circumstances $L_{WN}(443)$ may be close to the noise equivalent radiance of SeaWiFS. In principle $K_d(490)$ can be estimated from other ratios and hence the algorithms test for the estimated chlorophyll and use band ratios of higher wavelengths to achieve increased accuracy.

If chlorophyll < t_1 mg.m^{-3} then

$$\ln[K_d'] = A_1 + B_1 \ln[L_{WN}(443)/L_{WN}(555)]$$

If chlorophyll ≥ t_1 mg.m^{-3} and chlorophyll < t_2 mg.m^{-3} then

$$\ln[K_d'] = A_2 + B_2 \ln[L_{WN}(490)/L_{WN}(555)]$$

If chlorophyll > t_2 mg.m^{-3} then

$$\ln[K_d'] = A_3 + B_3 \ln[L_{WN}(510)/L_{WN}(555)]$$

The configurable thresholds t_1 and t_2 are set to 3 and 10 mg m^{-3} respectively. Values for A_1, B_1, A_2, B_2, A_3, B_3, are –2.30261, –1.29966, –1.574, –1.985, –1.541, and –3.209, respectively. All coefficients are read from the geophysical product configuration file and recorded in the CEOS leader file Geophysical Parameter Record.

Source: Personal communication from Dr Gerald Moore to Roland Flowerdew.

Validity: All water pixels.

Units: None (coefficient).

Range: 0.0 to 2.0.

3.4.3 ODOC algorithm

The ODOC algorithm is provides a measure of the dissolved organic carbon in the water. It is described in Aiken et al., 1995 [2]. Note that in that paper, ODOC is referred to as DOM, or dissolved organic matter. This algorithm is a band ratio, but of a different form:

$$\ln O = \alpha_0 + \alpha_1 \ln\left(\frac{L_{WN}(443)}{L_{WN}(490)}\right) + \alpha_2 \ln\left(\frac{L_{WN}(510)}{L_{WN}(555)}\right)$$

where O is the ODOC concentration; the α coefficients –0.021, 0.39 and –3.77 respectively (from Table 18 in Aiken *et al.*); and $L_{WN}(\lambda)$ the normalised water leaving radiances. Within SeaShark, the α coefficients are read from the geophysical product configuration file and recorded in the CEOS leader file, Geophysical Parameter Record. The bands used in the ratios are not configurable.

Source: The SeaWiFS CZCS-type pigment algorithm, [2].

Validity: All waters.

Units: mg m^{-3}.

Range: 0.01 to 5.0

3.4.4 PAR algorithm

The PAR algorithm calculates radiation available for photosynthesis on the basis of the atmospheric optical thickness (taking into account aerosol and ozone optical thickness).

This algorithm is almost entirely encapsulated within a look-up table, which is queried according to the values of three input parameters: the aerosol optical thickness (from the Wang correction), the aerosol Ångström-type exponent (calculated from the Wang aerosol epsilon ε as shown below), and the column integrated ozone (from the ancillary data). The exponent is given by $A = (\ln\varepsilon)/(\ln[765/865])$.

The interpolated result from the table is then processed according to the following equation to yield the PAR:

$$\mathrm{PAR} = \mathrm{PAR}_{table} d \cos\theta_{solar}$$

where θ_{solar} is the solar zenith angle and d is the Earth sun distance factor given in Volume 9 of the SeaWiFS Technical Report Series [12] as

$$d = \left[1 + 0.0167\cos\frac{2\pi(D-3)}{365}\right]^2$$ where D is the sequential day number of the year.

Source: The PAR table within SeaShark was generated by Dr Gerald Moore of the Plymouth Marine Laboratory according to [5].

Validity: The PAR algorithm is dependant upon the results of the atmospheric correction, and is applicable over all waters.

Units: µmol photon s^{-1} m^{-2}

Range: 0 to 4000.0.

3.4.5 Coccolithophore algorithm

The coccolithophore algorithm is based on a threshold band ratio test, and, if this is passed, the suspended sediment is likely to be coccolith in origin, and the value is copied into the coccolith output. (Note that a sediment value only occurs in case 2 waters.)

If $\rho_{443}/\rho_{555} > 0.9$, then set coccolith. The threshold is read from the geophysical product configuration file, and recorded in the CEOS leader file, Geophysical Parameter Record.

Source: Personal communication from Dr Gerald Moore to Roland Flowerdew.

Validity: Values may only be set in case II waters. Not valid in case IIy waters.

Units: g m^{-3}.

Range: 0.1 to 100.0.

3.4.6 Colour composite algorithm

The colour composite algorithm is a 15-bit representation of the top of atmosphere radiances of three channels set via the configuration file. (Usually, channels 6, 5 and 2 will be selected since these correspond to red, green and blue wavelengths.) Each channel is allocated 5 bits; the most significant bit is left blank. The maximum and minimum value for each channel is configurable, and the results are scaled between the maximum and minimum to ensure optimum representation. Additionally, each channel may be then weighted to decrease the effect on the overall result.

For each channel, the algorithm is the following:

$$\text{Result} = 32 \times \frac{\text{value} - \text{Minimum}}{\text{Maximum} - \text{Minimum}} \times \text{Weighting}$$

where Weighting is constrained to lie between 0.0 and 1.0, and Result is also constrained so it may not take the value of 32.0.

Result is then mapped to an integer; the full value for the three channels being obtained by the following integer calculation:

$$\text{Composite} = \text{Result}_{\text{channel 1}} + (32 \times \text{Result}_{\text{channel 2}}) + (1024 \times \text{Result}_{\text{channel 3}}) \ .$$

All coefficients are read from the geophysical product configuration file and recorded in the CEOS leader file, Composite and Irradiance Record.

Source: VEGA Group PLC.

Validity: All pixels. The colour composite is unaffected by fatal flags.

Units: None.

Range: Each channel may take integer values between 0 and 31.