

Change of the OSOAA implementation from version 1.6 to version 2.0

February 28th 2025

Note: the parameter CTE_STD_PRESSURE in OSOAA.h has been renamed CTE_DEFAULT_PRESSURE.

Change 1: Change in the wavelength in the medium “water” (“wavelength anomaly”)

Anomaly :

The wavelength used to estimate the radiative properties of Mineral-Like Particles in the sea water (phase function, scattering and extinction cross sections) and the phase function of Phytoplankton is the wavelength in the air, while it must be the wavelength relative to the medium “water”.

Evolution :

The wavelength λ_{sea} used to calculate the radiative properties of oceanic particles in the water medium is determined as follows:

$$\lambda_{sea} = \frac{\lambda_{air}}{m_{sea}}$$

where

- λ_{air} is the wavelength of simulation relative to the medium “air” (as defined by the user for a given simulation with -OSOAA.Wa)
- m_{sea} is the refractive of the seawater with respect to the air (defined by the user with -SEA.lnd)

The wavelength λ_{sea} is passed as an argument of the OSOAA_HYDROSOLS function to calculate the radiative properties of Phytoplankton and Mineral-Like Particles from the Mie Theory, accounting for their size distributions and refractive indexes.

The resulting data are stored in files defined by -PHYTO.ResFile and -MLP.ResFile (or the default names defined respectively by CTE_DEFAULT_FICGRANU_PHYTO and CTE_DEFAULT_FICGRANU_MLP in the file inc/OSOAA.h).

Let’s remind :

- the file -PHYTO.ResFile provides the phase function of the phytoplankton (decomposed in coefficients of the expansion into Legendre functions). The scattering and extinction cross-sections, obtained from the Mie Theory, are reported in this file as an additional information. Note, however, that the scattering and absorption coefficients for the phytoplankton that are really used to compute the radiance are calculated using the bio-optical empirical relationships derived from literature (equations 45 and 46 in the User Manual V1.2).
- the file -MLP.ResFile provides the phase function of the Mineral-Like Particles (Coefficients of the expansion into Legendre functions); the scattering and extinction cross-sections which are really used to calculate the scattering and absorption coefficients for the Mineral-Like Particles are calculated using bio-optical empirical relationships (equations 47 to 50 in the User Manual V1.2).

Analysis of the influence of the “wavelength anomaly” on the computations

Influence of the anomaly on the computation of the phase functions of hydrosols:

The phase functions simulated for the phytoplankton and the Mineral-Like Particles are provided from log files for both versions V1.6 and V2.0 of OSOAA.

The conditions of computations that were tested are:

- Phytoplankton scattering properties:
 - Junge power law size distribution:
slope (Junge exponent) = 4, $r_{\min} = 0.01 \mu\text{m}$, $r_{\max} = 200 \mu\text{m}$
 - Refractive index = 1.05
- Mineral-Like Particles scattering properties:
 - Junge power law size distribution: slope = 4, $r_{\min} = 0.01 \mu\text{m}$, $r_{\max} = 200 \mu\text{m}$
 - Refractive index = 1.15
- The wavelength for simulation is 440 nm in the air.

Figure 1 and Figure 2 show the phase functions (element P11 of the scattering matrix, which is informative on the Intensity) for the phytoplankton and the Mineral-Like Particles for both OSOAA versions V1.6 (blue line) and V2.0 (orange line, overlapping the blue line). Note that the y-axis is in log-scale on the left side of the graph. The green line shows the relative differences in percent (the corresponding y-axis is placed on the right side of the graph).

The phase functions (P11) are similar between version V1.6 and V2.0. The relative differences are lower than 0.3%. We also observe similar polarized phase functions (element P12 of the scattering matrix) (Figure 3 and Figure 4).

Therefore, the “wavelength anomaly” that does exist in version V1.6 of OSOAA has no impact on the directional distribution of the light propagation, including for the polarization component, regardless of the composition of the hydrosols (i.e., biogenic or minerals).

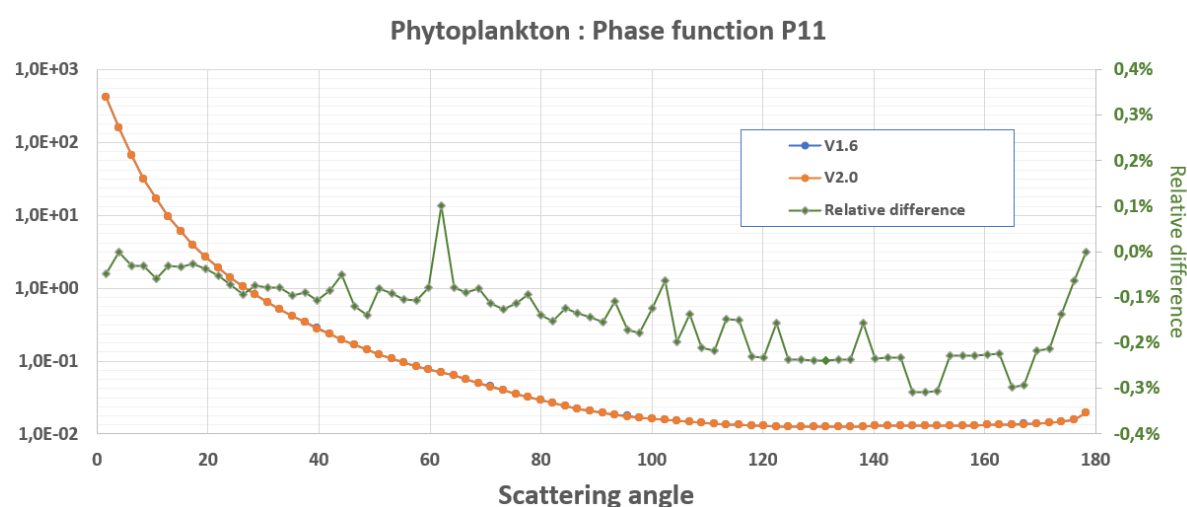


Figure 1 : phase functions of phytoplankton for OSOAA version V1.6 (blue line, left axis) and version V2.0 (orange line and left y-axis), and relative difference (green line and right y-axis).

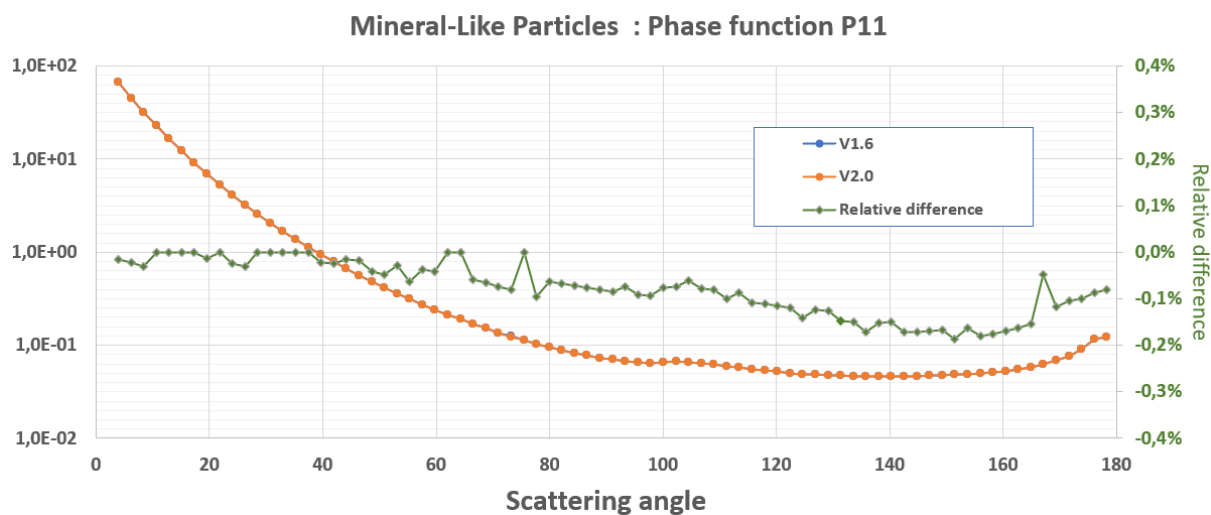


Figure 2 : phase functions of Mineral-Like particles for OSOAA version V1.6 (blue line and left y-axis) and version V2.0 (orange line and left y-axis), and relative difference (green line and right y-axis).

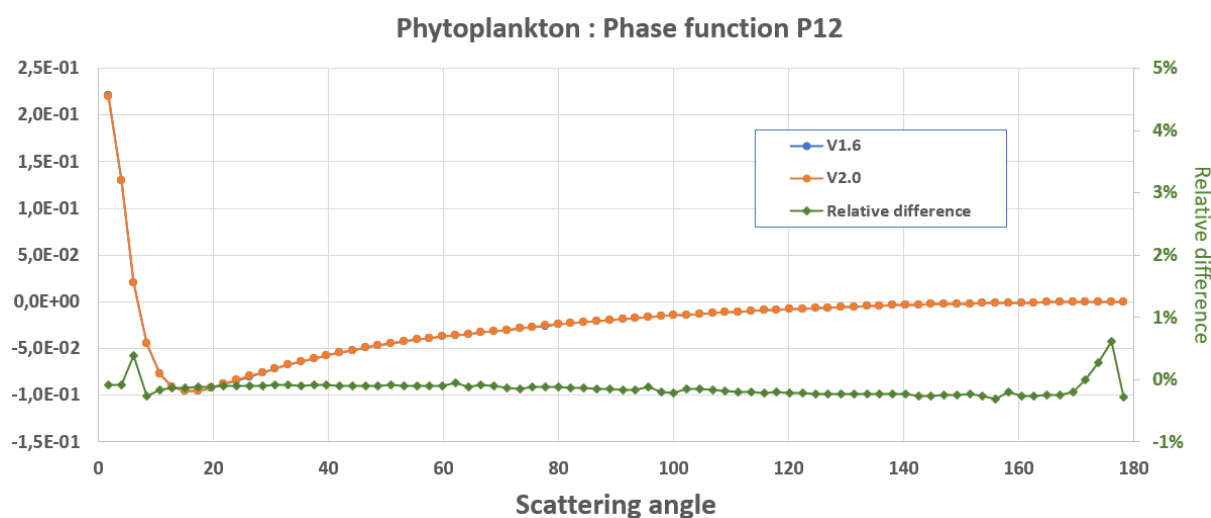


Figure 3 : polarized phase functions of phytoplankton for OSOAA version V1.6 (blue line and left y-axis) and version V2.0 (orange line and left y-axis), and relative difference (green line and right y-axis).

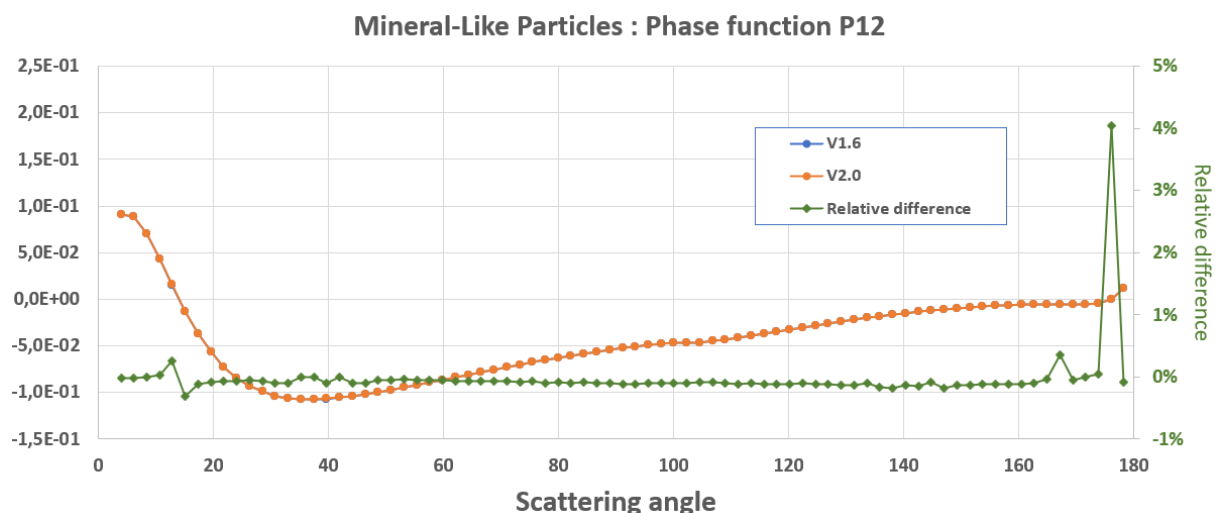


Figure 4 : polarised phase function of Mineral-Like particles for OSOAA version V1.6 (blue line and left y-axis) and version V2.0 (orange line and left y-axis), and relative difference (green line and right y-axis).

Influence of the anomaly on the calculation of cross-sections:

The scattering coefficient for phytoplankton (and consequently the cross-section for phytoplankton) is not impacted by the correction, because it is calculated from a bio-optical relationship which depends on the wavelength in air, as previously used.

On the other hand, the cross-section for the Mineral-Like Particles is impacted by the “wavelength anomaly”. Table 1 shows the cross-section is increased by about 35% in the simulated case in v2.0 relatively to v1.6. Such a change is somehow equivalent to perform a simulation using v1.6 with an increased concentration of Mineral-Like Particles of 35%.

Table 1 : radiative parameter from Mie calculations for Mineral-Like Particles for the versions V1.6 and V2.0 of OSOAA.

Radiative parameter	Value for V1.6	Value for V2.0	Relative difference
EXTINCTION CROSS SECTION (μm^2)	8,18E-05	1,10E-04	35,1%
SCATTERING CROSS SECTION (μm^2)	8,18E-05	1,10E-04	35,1%
ASYMMETRY FACTOR (no truncation)	8,81E-01	8,81E-01	0,0%
MEAN PARTICLES ALTITUDE/DEPTH (m)	-999	-999	0,0%
VOLUME OF A MEAN PARTICULE (μm^3)	1,24E-04	1,25E-04	0,8%
MEAN REFRACTIVE INDEX (real part)	1,15	1,15	0,0%
TRUNCATION COEFFICIENT	0,51384	0,51399	0,0%
SINGLE SCATTERING ALBEDO (truncation)	1	1	0,0%

Influence of the anomaly on the calculation of radiance:

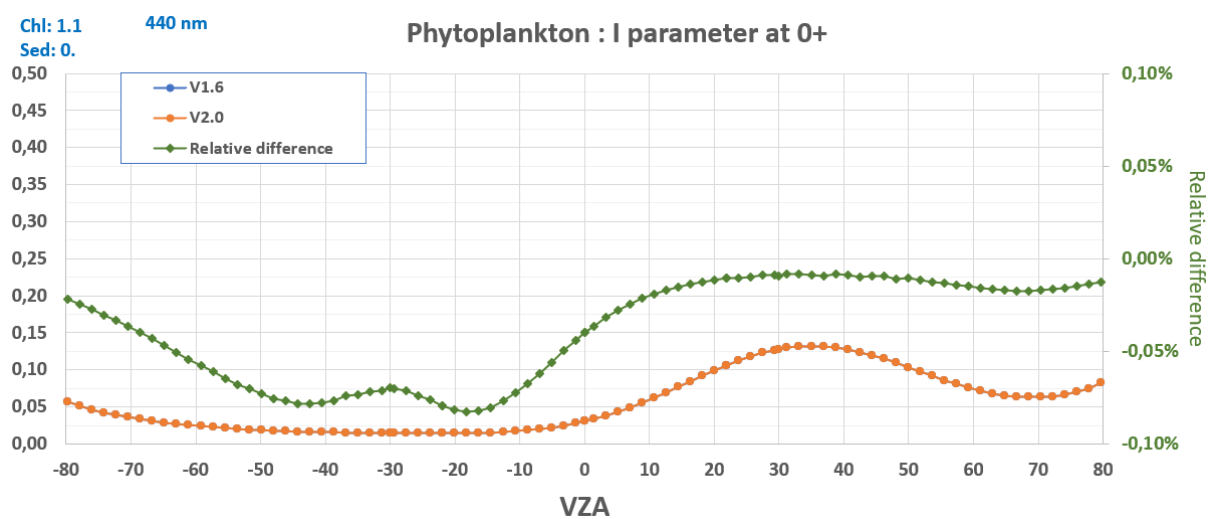
We assess the impact on radiance for the following conditions:

- At 440 nm
- The Sun Zenith Angle is 30°
- Aerosols: Shettle & Fenn Maritime model for 98% of relative humidity, with an AOT = 0.1 at 550 nm
- Phytoplankton concentration: 0 or 1.1 mg/m³
- Mineral-Like Particles concentration: 0 or 10 mg/ℓ
- Sea conditions: wind = 7m/s, air/sea index = 1.34
- Seabed depth at 1000 m.

Results when the concentration of Mineral-Like Particle is zero:

For a simulation without Mineral-Like Particle, **the scene is dark**.

Figure 5 shows that the impact of the correction is negligible: no more than 0.1% of difference for the intensity and no more than 0.03% of difference for polarized light.



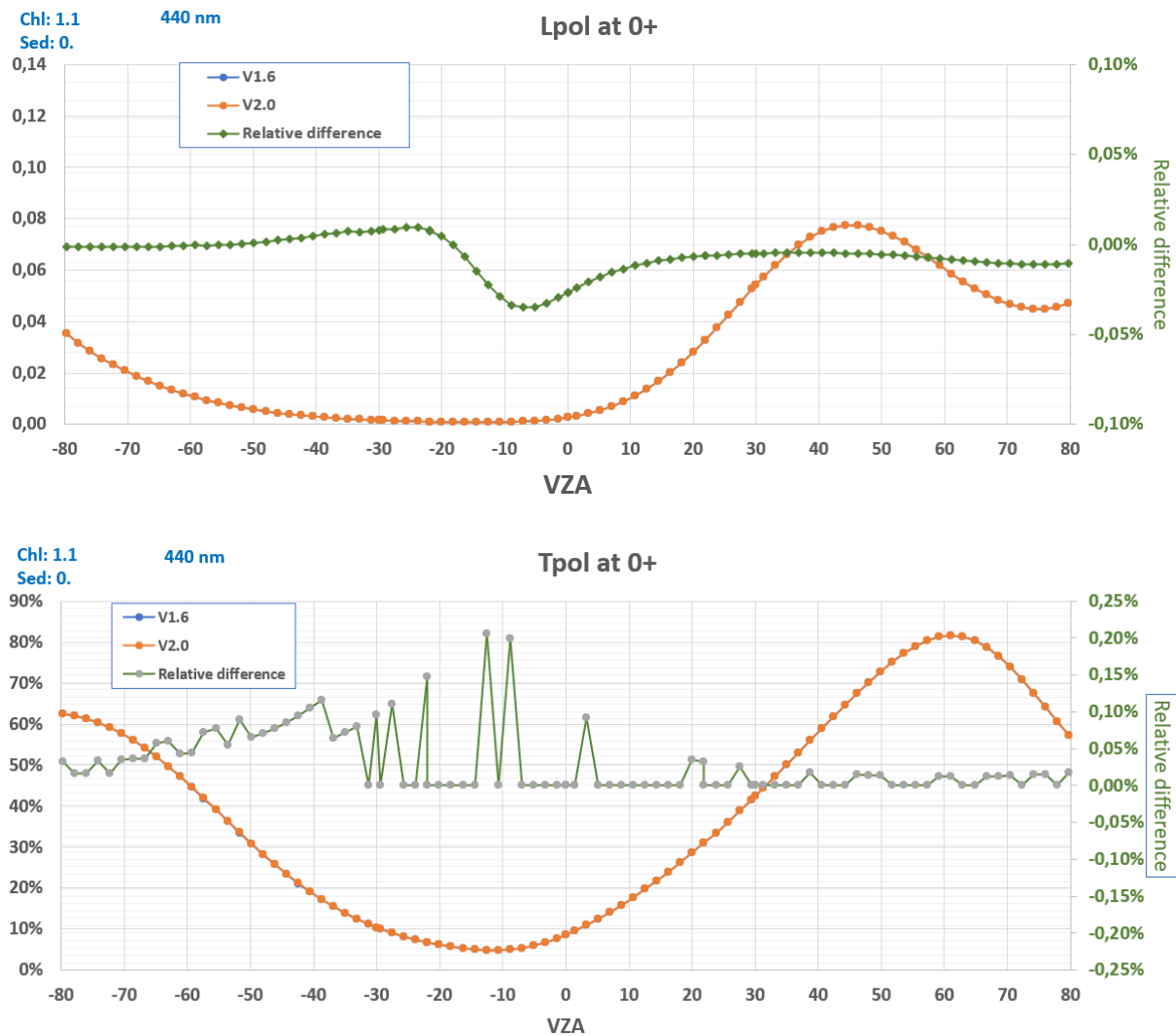


Figure 5 : Impact of the seawater wavelength correction for the case there is no Mineral-Like Particles but phytoplankton (1.1 mg/m³). Radiance normalised to the solar irradiance (I Stokes parameter), normalised polarized radiance and degree of polarization as a function of the viewing zenith angle, for the upward light at level 0+. OSOAA version V1.6 (blue line and left y-axis) and version V2.0 (orange line and left y-axis), and relative difference (green line and right y-axis). Note that the orange line is fairly overlapping the blue line.

Results when the concentration of Phytoplankton is zero:

For a simulation for which the concentration of Mineral-Like Particle is different from zero, **the scene is bright**.

Figure 6 shows that the impact of the correction is higher than that of the phytoplankton-only case:

- the impact on the intensity is about 2 – 2.5%,
- for polarized light, the impact is between 0 to 2% when the degree of polarization is far from zero (mainly around the sunglint spot). The impact is higher when the degree of polarization is weak. Note that relative impact is not relevant when polarization is almost zero, due to division by a very small number. This is the case for the highest values of relative impact, which are obtained for angles corresponding to almost zero polarization.

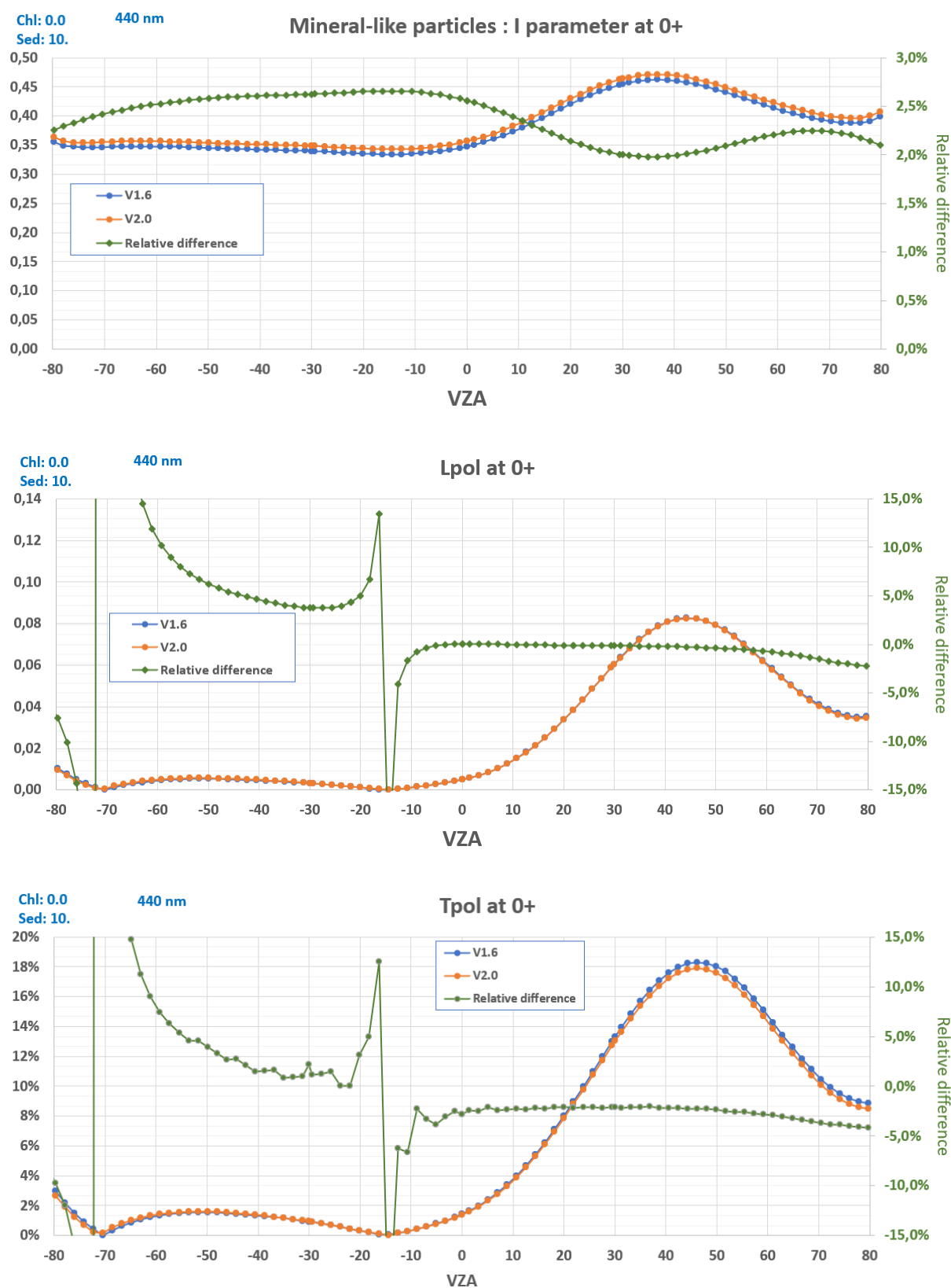


Figure 6 : Impact of the seawater wavelength correction for the case where the concentration of phytoplankton is zero and the concentration of Mineral-Like Particles is 10 mg/ℓ.

Change 2: Minor syntax modifications

Need :

The reading of output files can be altered by the occurrence of non “utf-8” characters. Such issues were solved as follows.

Modifications:

- In the routine OSOAA_SOS.F, the comment about the azimuth angles convention is changed. The symbol “°” used for degrees has been replaced by the explicit expression “degrees”. Practially, the following highlighted text:

Relative azimuth convention:

180° <-> Satellite and Sun in the same half-plane

0° <-> Satellite and Sun in opposite half-planes with respect to the zenith direction

has been replaced by the following highlighted text:

Relative azimuth convention:

180 degrees <-> Satellite and Sun in the same half-plane

0 degree <-> Satellite and Sun in opposite half-planes with respect to the zenith direction

Change 3: Option to switch off the polarization effects

Need : The users could need to perform simulations by ignoring the polarization effects (i.e., scalar radiative transfer model such as Hydrolight).

Modifications:

- A new constant parameter, named CTE_POLAR_SWITCHED_OFF, is introduced in the OSOAA.h file (in inc/).
- If CTE_POLAR_SWITCHED_OFF is 1, the polarization is not simulated. Note that a compilation of the OSOAA code is necessary to take into account the change of the value of this parameter. Such a polarization switch-off mode selection implies that:
 - the scattering coefficients for the polarization are set to 0 in OSOAA_SOS_CORE.F
 - the reflexion and polarization terms are set to 0 in OSOAA_SOS_CORE.F, both for a rough or flat sea surface.
 - the direct reflexion and transmission terms for the polarization are also set to 0 in OSOAA_TRPHI.F.
- the User Guide (user manual) has been updated to introduce the CTE_POLAR_SWITCHED_OFF in Table 1.

Change 4: Correction of the impossibility to change the number of Gauss angles applied to the calculation of phase functions.

Anomaly :

It was observed that setting the optional parameter -ANG.Mie.NbGauss by a value different than the default value in OSOAA.h (CTE_DEFAULT_NBMU_MIE) led to an error "OSOAA_ANGLES : ERROR_1020" and stopped the process.

Correction:

The calculation of the order of Fourier expansion $OS_{NM} = OS_{NB} + OS_{NS}$ is modified to be performed for two distinct cases:

- 1) the case of the use of the default value CTE_DEFAULT_NBMU_MIE
- or 2) the case of the use of the user value -ANG.Mie.NbGauss.

Change 5: Adding the option “HYD.Model=3” to allow using a user’s defined marine profile of absorption and scattering coefficients, coupled with a user’s defined Mueller matrix

Need :

The version V1.6 of OSOAA is able to take into account a user-defined external Mueller matrix of hydrosols. This corresponds to the following option: **HYD.Model=2**. The absorption and scattering coefficients are then calculated by applying bio-optical empirical relationships (taken from literature) that link the chlorophyll concentration with the absorption/scattering coefficients of the phytoplankton. In this way, a user-defined external phase function (such as those that could be measured in the field) is related to the scattering microphysical properties (e.g., scattering and absorption cross-sections) derived from Mie theory rather than from user’s field measurements. Note also that the user-defined external phase function is ascribed to the phytoplankton component of the hydrosols in V1.6 and not to the “mineral-like” particle component of the hydrosols.

The version V2.0 of the OSOAA model permits the introduction of a user-defined external Mueller matrix of hydrosols that is directly related to a user-defined vertical profile of absorption and scattering coefficients in the water column such as a profile that is based on field measurements of the inherent optical properties of the hydrosols.

Modifications:

The objective was to adjust the OSOAA model without complexifying the code.

The option **HYD.Model=3** is then introduced to allow the use of a user-defined external Mueller matrix of hydrosols together with a user-defined vertical profile of absorption and scattering coefficients of the hydrosols within the water column.

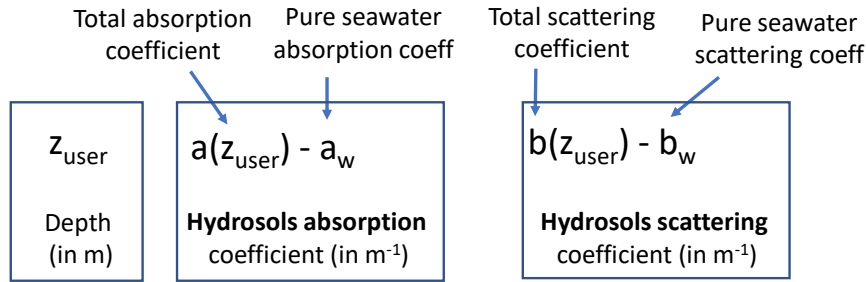
The inputs required by such a new option are as follows:

- **HYD.ExtData**, which is a file that aims at providing the user-defined external Mueller matrix (such an input already exists in the OSOAA version V1.6)

Ω	$F_{11}(\Omega)$	$(-F_{12}/F_{11}) (\Omega)$	$(F_{22}/F_{11}) (\Omega)$	$(F_{33}/F_{11}) (\Omega)$
Scattering angle (in °)	Phase function in intensity			

The phase function F_{11} data (unit: sr^{-1}) is defined as the Volume Scattering Function (**VSF, unit: $\text{m}^{-1}\text{sr}^{-1}$**) **normalized by the scattering coefficient b (unit: m^{-1})** (both measured just beneath the sea surface). The polarization terms (F_{12} et F_{33}) are also in unit sr^{-1} . The assumption of a spherical shape of the hydrosols is implicitly made in the OSOAA model (Mie theory).

- An additional input file **HYD.UserProfile** that provides the user measured vertical profile of absorption and scattering coefficients of hydrosols in the water column.



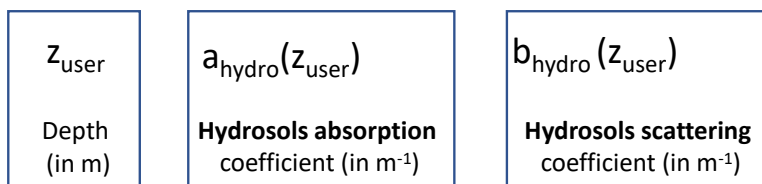
Note that the pure seawater absorption and scattering coefficients (respectively a_w and b_w) are supposed to have been subtracted from the native user's measurements $a(z_{\text{user}})$ and $b(z_{\text{user}})$.

The changes in the OSOAA program to implement the new option **HYD.Model = 3** concern the OSOAA_MAIN routine by introducing the definition of the file **HYD.UserProfile** and the subroutine OSOAA_PROFILE by introducing two new arguments: the new user profile file and the parameter IMOD_HYD which provides the value of the option **HYD.Model**.

The handling of the option **HYD.Model = 2** in OSOAA_MAIN is extended to the case **HYD.Model = 3** by assigning the optical properties of the hydrosols (absorption coefficient, scattering coefficients and Matrix elements) artificially to Phytoplankton component of the hydrosols, thus the optical properties of Mineral-like particles (MLP) are set to zero including its phase matrix.

The subroutine OSOAA_PROFILE needs to be modified as follows to take into account the case **HYD.Model = 3**:

- The user's profile of absorption and scattering coefficients is read for the given user's depth values (z_{user}):



If the user's profile does not reach the seabed or the depth limit calculated by the OSOAA code (corresponding to the maximum optical thickness CTE_SEA_T_LIMIT), then the absorption and scattering coefficients are duplicated below the deepest layer of the user's profile till the depth limit.

Note: the maximum number of lines of the user's file should be lower than CTE_NZ_MAX_USER_PROFILE (new constant value defined in OSOAA.h).

- The vertical resolution of the profile (i.e., depth step) specified by the parameter CTE_SEA_DEPTH_STEP (in meter) is obtained using interpolations of user's depth initial measurements (note that the depth resolution, which is defined in inc/OSOAA.h, is 0.05 m by default). The profile of absorption and scattering coefficients for depths z_{OSOAA} is then obtained as follows:

z_{OSOAA}	$a_{\text{hydro}}(z_{\text{OSOAA}})$	$b_{\text{hydro}}(z_{\text{OSOAA}})$
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- The scattering mixing rate for hydrosols is then calculated for each depth z_{OSOAA} as follows:

$$pc_{\text{phyto}}(z_{\text{OSOAA}}) = \frac{b_{\text{hydro}}(z_{\text{OSOAA}})}{[a_{\text{hydro}}(z_{\text{OSOAA}}) + a_w] + [b_{\text{hydro}}(z_{\text{OSOAA}}) + b_w]}$$

Hydrosols scattering coefficient (in m^{-1})

Total extinction coefficient (in m^{-1}) including the pure seawater

The scattering mixing rate for hydrosols is assigned to the phyto parameter (by convention)

The scattering mixing rate is artificially assigned to the component pc_{phyto} (mixing rate of phytoplankton) and the component pc_{MLP} (mixing rate of Mineral Like-Particle) is set to zero for all the depth levels. In the same way, the phase matrix is assigned to the Phytoplankton component of the hydrosols and the matrix for Mineral-like particles is set to zero. The pure seawater absorption and scattering coefficients (respectively a_w and b_w) are introduced. They do not depend on the depth but only on the wavelength. The related parameters are obtained according to equations and data given in §4.3.3.2, of the version V2.0 of the user manual.

- The scattering mixing rate for the pure seawater is also calculated for each depth:

$$pc_w(z_{\text{OSOAA}}) = \frac{b_w}{[a_{\text{hydro}}(z_{\text{OSOAA}}) + a_w] + [b_{\text{hydro}}(z_{\text{OSOAA}}) + b_w]}$$

Pure seawater scattering coefficient (in m^{-1})

The scattering mixing rate for a given component (seawater molecules, phytoplankton or Mineral-Like Particles) is defined as the ratio between the scattering coefficient of the given component and the total extinction coefficient (absorption + scattering for all the components). These scattering mixing rates are directly used to weight the Mueller matrix of each hydrosol component (Phytoplankton, water, Mineral-Like particles) for computing the directional scattering properties of the light propagating in medium through $pc \times F11(\Omega)$.

- The total extinction optical thickness is calculated as follows:

$\tau_{\text{ext}}(z_p) = \sum_{k=0}^p [a(k) + b(k)] \times \Delta z(k)$ where p is the index of the OSOAA profile level corresponding to the depth z_p , and for $a(k)$ and $b(k)$ respectively the total absorption and total scattering coefficients at the depth level k (see Figure 7 which illustrates the sea profile definition).

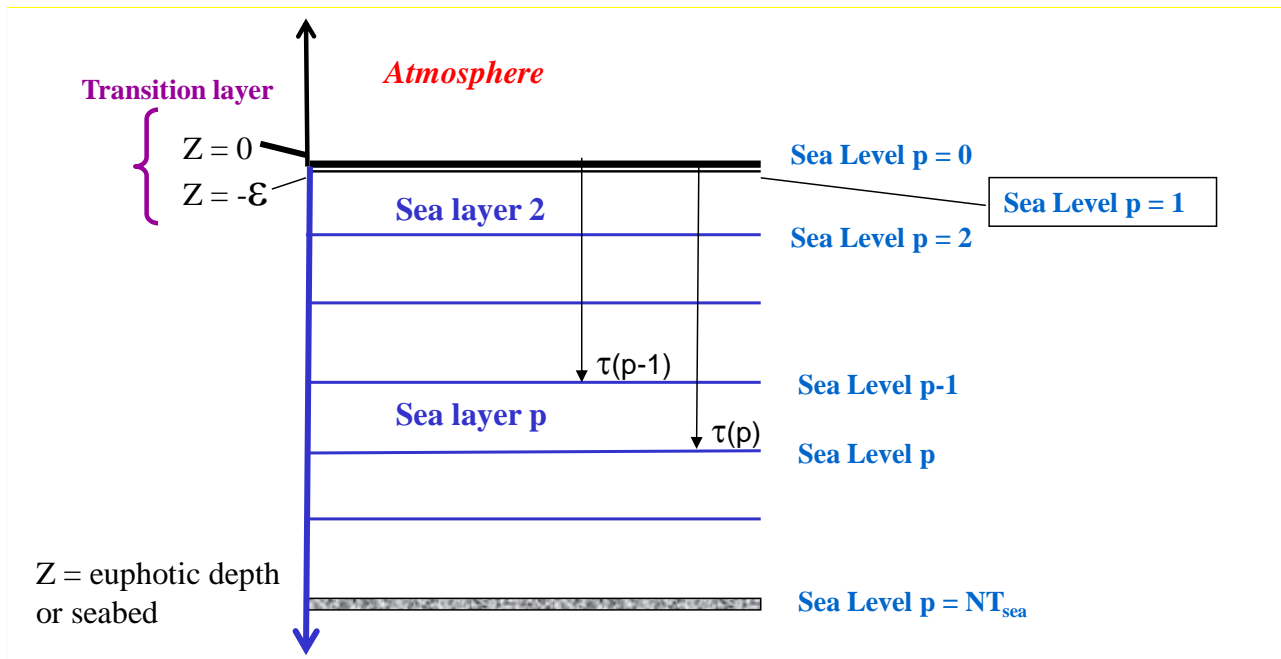


Figure 7 : Illustration of the sea profile definition

We then get the profile for the optical thickness profile of the OSOAA model, as shown below:

Level p	z	τ_{ext}	pc_{mol}	pc_{phyto}	$pc_{MLP} = 0$
Level number of the profile	Sea depth (in m)	Total optical thickness at level p	Scattering mixing rate for pure seawater	Scattering mixing rate for hydrosols	
No dimension					

The implementation of the vertical profile of the hydrosol optical properties (routine OSOAA_PROFILE) remains similar in V2.0 as it was performed in the V1.6 version when **HYD.Model** $\neq 3$.

A new constant value is introduced in the inc/OSOAA.h file:

```
Maximum number of depth values in the user profile of absorption and
scattering coefficients
CTE_NZ_MAX_USER_PROFILE          500
```

Change 6: Adding a consistency test for the case of “HYD.Model=2” (user-defined external Mueller matrix using a vertical profile of absorption and scattering coefficients defined for phytoplankton component, using Mie theory)

Anomaly :

It was observed that the setting of the optional parameter -SED.Csed with a non-zero value when using the option -HYD.Model=2 (which corresponds to the case for which the Mueller matrix is provided by the user, but the profile of absorption and scattering coefficients is defined according to the phytoplankton parameters based on Mie theory) leads to “Nan” values in the vertical profile of the inherent optical properties of the hydrosols and subsequently in the radiance simulation outputs.

Correction:

Indeed, the case -HYD.Model=2 can only consider the case for which the Mueller matrix is defined for phytoplankton.

A new test of the input parameters has been introduced in the OSOAA_MAIN routine to check that the parameter -SED.Csed is set to zero when -HYD.Model is 2.

Change 7: Correction of a column overflow

Anomaly :

It was noticed in the source code of subroutine SOS_DECOMPO_LEGENDRE, included in the file SOS_PARTICLES_RAD.F, a column overflow (i.e., column 73 was used for one line, obviously without impact on the simulations) for the calculation of the slope of the truncated part of the phase function. Note that there is no issue with the computation (test for a compilation by gfortran).

Correction:

The calculation is now split into two lines to only use columns 7 to 72, as required by Fortran 77 compiler.

Change 8: Change of the flux values provided by OSOAA

Anomaly :

The OSOAA outputs provide values of radiance I that are normalized to the solar irradiance:

$$I = \frac{\pi}{E_s^V} \cdot L(E_s^V) \text{ where } L(E_s^V) \text{ is the real radiance for the real solar irradiance } E_s^V.$$

The conversion from normalized radiance to real radiance can be done by multiplying the OSOAA radiance outputs by the coefficient E_s^V / π (considering that the user is supposed to provide the real solar irradiance E_s^V).

On the other hand, the fluxes provided in V1.6 were calculated for radiance that are normalized to the solar irradiance with an additional division by π . Therefore, the conversion of OSOAA outputs (i.e., normalized) fluxes into geophysical fluxes (i.e., not normalized) could be done by only multiplying with the real solar irradiance E_s^V .

As the conversion factor is not the same for radiance and flux, this can lead to confusion.

Note that the OSOAA code correctly handled the π normalization of fluxes in version V1.6 when using fluxes data in radiative transfer calculations. There were therefore no anomalies in the radiance, reflectance and polarization results from a physical point of view.

Correction:

For OSOAA V2.0, the values of flux provided in log files are expressed in terms of flux for normalized radiance calculated using a solar irradiance equals to π , without an additional division by π . This is the same for the content of the flux file (flux.txt).

By this way, the conversion of fluxes provided by OSOAA into geophysical fluxes (i.e., not normalized), and the conversion of normalized radiance into real radiance, can be done by using the same coefficient E_s^V / π .

Adjustment of comments were made in the result files accordingly.

Adjustments of the user manual were made accordingly.

Note:

In addition, the file format has been modified to expand the exponents using 3 digits (rather than 2) to allow writing values of flux lower than 10^{-100} and avoid simulation failures.

```
600 FORMAT(2X,I4,1X,F12.5,2X,7(2X,E12.6))
```

has become:

```
600 FORMAT(2X,I4,1X,F12.5,2X,7(2X,E14.6E3))
```

Change 9: Reprocessing without changing the bio-optical conditions of a given simulation

Anomaly :

In the case for which the user performs the same simulations but desires an output for a different relative azimuth angle relatively to the initial inputs or for a different viewing angle or a different level in the profile, without any changes in the bio-optical input parameters, the full radiative transfer calculation should not be repeated entirely to save a lot of time. The previous result file, including the radiance field for all the directions and levels of the profile, needs to be re-used to save significantly the computing time. However, in some cases, it was observed that the full radiative transfer calculation is reprocessed:

- If the OSOAA.h is modified after processing: the first reprocessing (after a new compilation) is identified as a change of conditions, as expected, but a second reprocessing without any change of parameters is abnormally considered as a new one.
- If the parameter -SED.JD.rmin is defined as the default value in OSOAA.h, it is abnormally considered as a change.
- If the parameter -YS.Swa or DET.Swa is defined in the command line using their default values, as defined in the OSOAA.h file, then it is abnormally considered as a change.

Correction:

- The file exe/config.txt (copy of inc/OSOAA.h, made during the compilation) is now copied in the results repository even if it is not the first time the results are written in this directory. This corrects the fact that this file was not updated in the simulation results repository for OSOAA version V1.6.
- The default value for the parameter -SED.JD.rmin (which is the minimum radius for a size distribution of Mineral-Like particles defined by the Junge model) in the inc/OSOAA.h file (CTE_DEFAULT_HYD_JUNGE_RMIN) was defined as 0.01 (float value). However, the value that is read by the program may be very slightly different (by an order of magnitude of 10^{-9}). This can be corrected by defining a double precision value in the inc/OSOAA.h file:
`CTE_DEFAULT_HYD_JUNGE_RMIN 0.01D+00`

Note, however, that such a way of addressing the issue leads to an anomaly in the use of the GUI (Graphical Unit Interface). Therefore, a solution based on a comparison between the value of each parameter in the current process and the value in the previous process is used. The comparison is based on an absolute difference threshold, which is set to 1.D-06 to be consistent with the encoding values in the ListParam.txt file.

- In the case for which the parameter -YS.Swa or -DET.Swa are not defined by the user, their default values are assigned in the subroutine OSOAA_PROFILE.F. Since the assignment is made after the comparison of the current simulation parameters to those of the previous simulation, that means the parameters -YS.Swa or DET.Swa are still undefined (i.e. they have the value CTE_NOT_DEFINED_VALUE_DBL given in inc/OSOAA.h) to compare their values between the two successive simulations. Therefore, even if the previous simulation was made with a

definition of the parameters -YS.Swa and -DET.Swa given by the user with the default values, they are considered as different for the reprocessing.

This has been corrected by assigning the default values in the routine OSOAA_MAIN.F at the initialization phase of the various parameters. The change impacts also the subroutine OSOAA_PROFILE.F.

The default values in inc/OSOAA.h are now also given in the double precision format.

Change 10: Clarification of parameters to define a gaussian vertical profile of chlorophyll

Anomaly :

In the OSOAA version V1.6, the gaussian vertical profile of chlorophyll concentrations is given for the simulation case **-PHYTO.ProfilType 2** as follows:

$$\text{Chl}(z) = C_1 + C_0 \cdot \exp\left(-\frac{(z - z_{\max})^2}{2\sigma^2}\right)$$

where the parameters are defined by the user as follows:

- C_0 : the chlorophyll-a concentration at the sea surface (**PHYTO.Chl**, in mg.m^{-3}).
- C_1 : the constant background biomass (**PHYTO.GP.Chlbg**, in mg.m^{-3}).
- Z_{\max} : the depth for which the chlorophyll-a concentration is maximum (**PHYTO.GP.Deep**, in m)
- σ : the width of the chlorophyll peak of the Gaussian function (**PHYTO.GP.Width**, in m)

The parameter **PHYTO.Chl** is also used to define a homogeneous profile, for the simulation case **-PHYTO.ProfilType 1**:

$$\text{Chl}(z) = C_0 \quad \text{with } C_0 \text{ the chlorophyll-a concentration at the sea surface.}$$

Using the same name of the parameter (**PHYTO.Chl**) for two different bio-optical values should be avoided as it can lead to confusion.

In addition, the C_0 factor is not the chlorophyll-a concentration at the sea surface in the case of a gaussian profile but the concentration at depth Z_{\max} where the Chl-a concentration is maximum.

Improvement:

- A new parameter, called (**PHYTO.GP.Chlzmax**, in mg.m^{-3}) is introduced to define the maximum chlorophyll-a concentration of the gaussian profile that is reached at the depth when $Z = Z_{\max}$

The gaussian profile is then given by:

$$\text{Chl}(z) = \text{Chl}_{bg} + \text{Chl}_{z_{\max}} \cdot \exp\left(-\frac{(z - z_{\max})^2}{2\sigma^2}\right)$$

where the parameters are defined by the user as follows:

- $\text{Chl}_{z_{\max}}$: the maximum chlorophyll-a concentration of the gaussian profile, that is reached for a depth $Z = Z_{\max}$ (**PHYTO.GP.Chlzmax**, in mg.m^{-3}).
- Chl_{bg} : the constant background biomass concentration (**PHYTO.GP.Chlbg**, in mg.m^{-3}).
- Z_{\max} : the depth for which the chlorophyll-a concentration is maximum (**PHYTO.GP.Deep**, in m)
- σ : the width of the chlorophyll peak of the Gaussian function (**PHYTO.GP.Width**, in m)

The new parameter **PHYTO.GP.Chlzmax** is introduced in the routine OSOAA_MAIN and in the GUI.

It is supplied to the subroutines OSOAA_PROFILE and OSOAA_SEA_PHY_COEFFS, both included in the file OSOAA_PROFILE.F.

Example for a practical case to show how to adapt a processing script from V1.6 to V2.0:

Considering the case for which the user wishes to simulate a gaussian chlorophyll profile from OSOAA that is defined as follows:

$$\text{Chl}(z) = 0.1 + 6 \times \exp\left(-\frac{(z - 40)^2}{2 \times 5^2}\right) \text{ mg. m}^{-3}$$

where z is in meters

For the version V1.6, the command line parameters would be as follows:

-PHYTO.ProfilType 2 \
-PHYTO.GP.Chlbg 0.1 -**PHYTO.Chl** 6. -PHYTO.GP.Deep 40. -PHYTO.GP.Width 5.

For the version V2.0, the command line will become:

-PHYTO.ProfilType 2 \
-PHYTO.GP.Chlbg 0.1 -**PHYTO.GP.Chlmax** 6. -PHYTO.GP.Deep 40. -PHYTO.GP.Width 5.

In the case of a simulation for a homogeneous chlorophyll profile, there is no change in the command line.

As an example, it will remain: -PHYTO.ProfilType 1 -PHYTO.Chl 4.

Change 11: Modification of parameter consistency tests

Anomaly :

The introduction of the possibility to use a user-defined profile of absorption and scattering coefficients (case **HYD.Model=3** with an associated file **HYD.UserProfile**) shows a strong impact on the consistency of the list of parameters. For instance, the definition of a concentration of chlorophyll or Mineral-Like particles together with a user-defined profile of absorption and scattering coefficients leads to confusion because it is not clear what parameters between the bio-optical absorption/scattering coefficients calculated based on empirical relationships from literature and the user-defined absorption/scattering coefficients (measurements) are actually being used.

Furthermore, it has been noticed that feeding the code with a user-defined profile of chlorophyll concentration (case **PHYTO.ProfilType=3** with the associated file **PHYTO.Userfile**) requires to define the chlorophyll concentration at the sea surface (**PHYTO.Chl**), even if the latter was not used. However, if the **PHYTO.Chl** concentration is set to zero, the profile is then forced to be homogeneous (with a zero concentration of chlorophyll). In this case, the use of the expected user-defined profile of chlorophyll concentration is then not considered.

Correction:

The consistency between all the parameters has been reviewed. Some warning messages are now provided in the case of an inconsistency between parameters.

The definition of **HYD.Model=3** (user-defined profile of absorption and scattering coefficients) is considered as a priority relatively to the definition of the hydrosol concentrations.

The steps involved in checking the parameters are as follows:

If **HYD.Model == 3**:

- Check that **HYD.ExtData** (Mueller matrix) and **HYD.UserProfile** (absorption and scattering coefficients profile) are defined,
- Display a warning message if the information on chlorophyll concentration profile is given since it is not supposed to be used.

Else:

If **HYD.Model == 1 or 2**:

- Check that the inputs related to yellow substance and detritus absorption properties are defined, as well as the inputs related to the mineral-like particles concentration.
- Check that the type of the vertical profile of chlorophyll (**PHYTO.ProfilType**) is defined.
- If **PHYTO.ProfilType == 3** :
 - Check that the file of chlorophyll concentration profile is defined.
 - Display a warning message if other information on chlorophyll concentration is given (homogeneous or gaussian profile definition), since it is not supposed to be used.
- If **HYD.Model == 1** : (Hydrosols radiative properties calculated by Mie calculation)

- If the chlorophyll concentration or mineral-like particles concentration is not zero, check that the repository for Mie result files is defined.
- If the chlorophyll concentration is not zero, check that the size distribution parameters for phytoplankton are defined.
- If the mineral-like particles concentration is not zero, check that the size distribution parameters for MLP are defined.
- If HYD.Model == 2 : (hydrosols optical properties provided by user-defined data)
 - Check that HYD.ExtData (Mueller matrix) is defined.
 - Check that the mineral-like particles concentration is zero (SED.Csed).

Else (HYD.Model not defined or $\neq 1, 2, 3$):

- Force parameters to be consistent in the case of pure seawater (no chlorophyll, neither mineral-like particles).

Change 12: New output files to provide IOP of hydrosols and aerosols

Need :

The information related to the Inherent Optical Parameters (e.g., absorption, scattering, backscattering coefficients) of hydrosols are provided in V1.6 within log files, which are not designed for an easy use and the IOP information is not clear visible because of the large amount of other pieces of information contained in the log-file. The users need to access easily to the information about the IOP of hydrosols (and aerosols) in a dedicated file.

Evolution:

New optional output files are introduced:

- **AER.ResFile.IOP** that provides the following IOPs for aerosols:
 - Extinction cross-section (in μm^2)
 - Scattering cross-section (in μm^2)
 - The single scattering albedo
 - The phase functions of the Mueller matrix (no truncation is applied) in sr^{-1} :
 - P11: for intensity
 - P12, P22 and P33 for the polarization elements.

The routine OSOAA_AEROSOLS has been adjusted to introduce the new parameter **AER.ResFile.IOP** using the optional keyword AER.ResFile.IOP (FICAER_IOP). The IOPs above mentioned are reported into the file AER.ResFile.IOP.

- **HYD.ResFile.IOP** that provides the following IOPs for hydrosols:

The scattering coefficient b (in m^{-1}) and the backscattering coefficient bb (in m^{-1}) are given by:

$$b = \frac{1}{4\pi} \int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi} VSF(\theta) \cdot \sin\theta \cdot d\theta \cdot d\phi = \frac{1}{2} \int_0^{\pi} VSF(\theta) \cdot \sin\theta \cdot d\theta$$

$$bb = \frac{1}{4\pi} \int_{\phi=0}^{2\pi} \int_{\theta=\pi/2}^{\pi} VSF(\theta) \cdot \sin\theta \cdot d\theta \cdot d\phi = \frac{1}{2} \int_{\pi/2}^{\pi} VSF(\theta) \cdot \sin\theta \cdot d\theta$$

where $VSF(\theta)$ is the volume scattering function.

(source: Ocean Optics Web Book, <https://www.oceanopticsbook.info/view/inherent-and-apparent-optical-properties/volume-scattering-function-vsrf>)

The volume scattering function is related to the phase function $p(\theta)$ as follows:

$$p(\theta) = \frac{VSF(\theta)}{b}$$

The normalization condition of the phase function within the OSOAA model is as follows: $\int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi} p(\theta) \cdot \sin\theta \cdot d\theta \cdot d\phi = 4\pi$

$$\text{i.e. } \int_0^\pi p(\theta) \cdot \sin\theta \cdot d\theta = 2$$

Note: other authors (e.g., Mobley, Ocean Optics Web Book) could consider a normalization condition of the phase function to 1, instead of 4π as used for OSOAA.

The OSOAA model calculates the scattering coefficient b of phytoplankton from bio-optical relationships derived from literature. The scattering coefficient for Mineral-Like Particles is calculated using Mie theory. The OSOAA model calculates the phase function for both types of hydrosols (phytoplankton and Mineral-Like Particles) using either Mie theory or user-defined data.

The backscattering coefficient is calculated by:

$$bb = \frac{b}{2} \int_{\pi/2}^\pi p(\theta) \cdot \sin\theta \cdot d\theta$$

The file containing the IOPs for hydrosols (**HYD.ResFile.IOP**) provides the phase functions of the Mueller matrix (no truncation is applied) in sr^{-1} :

- P11: for intensity
- P12, P22 and P33 for the polarization elements.

Such a file provides as well the vertical profile of coefficients b (in m^{-1}) and bb (in m^{-1}), and profile of the backscattering ratio bb/b . These IOPs are provided successively for phytoplankton and for Mineral-Like Particles. They are also provided for the mixing of these components in the medium, accounting for their relative mixing scattering rate and for the absorption by water molecules and CDOM.

To achieve this implementation, it was necessary to adjust the OSOAA_HYDROSOLS.F, OSOAA_PROFILE.F and OSOAA_MAIN.F source files. The routine OSOAA_HYDROSOLS.F has been adjusted to introduce the name of the IOP file as an input parameter, using the optional keyword **HYD.ResFile.IOP** (**FICHYD_IOP**); the phase functions are written into this file (**HYD.ResFile.IOP**). A new output parameter named "INT_90_180" is also introduced. It provides the value of the integration of the phase function from 90° to 180° (for a phase function which is normalized to 4π in space).

The routine OSOAA_PROFILE has been adjusted to provide new output results into the main program OSOAA_MAIN:

- The number of layer (NZ) of the marine vertical profile is given for the depth values (in m) in the table PROF_Z[0:CTE_NZ_MAX].
- The scattering coefficient of Mineral-Like Particles (SED_DIF) is supposed to be constant over all the profile (in m^{-1}).
- The vertical profile of scattering coefficients of phytoplankton (in m^{-1}) is given in the table PROF_PHY_DIF[0:CTE_NZ_MAX].
- The vertical profile of scattering coefficients for the overall medium (in m^{-1}) is given in the table PROF_Z_COEF_SCA[0:CTE_NZ_MAX].

- The vertical profiles of the scattering mixing rate for phytoplankton and for Mineral-Like Particles are respectively given in table PROF_Z_MEL_PHY[0:CTE_NZ_MAX] and table PROF_Z_MEL_SED[0:CTE_NZ_MAX].

The program OSOAA_MAIN has been adjusted to read the new optional keywords and to provide the associated values to the subroutines. For hydrosols, it writes information first for phytoplankton, secondly for Mineral-Like Particles and finally for the overall medium mixing particles. If a user-defined Mueller matrix is used for calculation (HYD.Model 2 or 3), the program OSOAA_MAIN provides the corresponding vertical profiles of b , bb and bb/b coefficient. The scattering coefficient profile is arbitrarily assigned to the phytoplankton component.

Change 13: Removal of IEEE_UNDERFLOW_FLAG IEEE_DENORMAL warning messages at the end of simulation processing

Need :

Some processes are finished with the warning message "IEEE_UNDERFLOW_FLAG IEEE_DENORMAL ". It is necessary to investigate the causes of this message.

Evolution:

Some calculations can generate very insignificant values. In that case, when the value is lower than the smallest encodable double precision value, we get the warning message: "IEEE_UNDERFLOW_FLAG IEEE_DENORMAL ". The value is considered as to be zero, without any impacts on the simulation.

Such a truncation to zero may appear in the routine OSOAA_GRANU (in OSOAA_PARTICLES_RAD.F) when calculating the Log-Normal size Distribution (LND), for very small values of radius r (and also for very large values of radius):

$$N^{\text{LND}}(r) = \frac{1}{r \cdot \sigma \cdot \sqrt{2\pi}} \times \exp\left(-\frac{\ln^2(r/r_m)}{2\sigma^2}\right)$$

where r_m and σ are respectively the modal radius and standard deviation of the size distribution

This warning can be avoided by finishing the main program by the command END rather than the command STOP. Such a modification was performed in the version 2.0 of the OSOAA_MAIN.F file.

Change 14: Clarification of used angles in logfiles for hydrosols and aerosols

Need :

The logfile -HYD.Log provides the list of cosines of Gauss angles (μ) which are used to calculate of phase function. The positive values μ allow covering the scattering angles from 0 to 90°. In addition, the 90° to 180° scattering angles are defined on the basis of the opposite values $-\mu$. However, they are listed in the log file as negative angles, rather than as scattering angles. This can be confusing for users.

The same applies to the aerosol logfile -AER.Log.

Evolution:

The OSOAA_HYDROSOLS.F and OSOAA_AEROSOLS.F source files are modified to list the angles as following:

- If $\mu > 0$, then the corresponding angle is $\text{acos}(\mu)$
- If $\mu < 0$, then the corresponding angle is $180 - \text{acos}(\mu)$

This modification concerns the “List of used angles: Index, mu, angle (degrees), weight” in the logfiles.

Example:

```
List of used angles :
Index, mu, angle (degrees), weight
-41 -0.10000000000000D+01 180.000 0.00000000000000D+00
-40 -0.99955382265163D+00 178.288 0.11449500031887D-02
-39 -0.99764986439824D+00 176.071 0.26635335895156D-02
-38 -0.99422754096569D+00 173.841 0.41803131246915D-02
-37 -0.98929130249976D+00 171.607 0.56909224514044D-02
.
.
.

-3 -0.97408398441585D-01 95.590 0.38839651059052D-01
-2 -0.58504437152421D-01 93.354 0.38958395962770D-01
-1 -0.19511383256794D-01 91.118 0.39017813656307D-01
1 0.19511383256794D-01 88.882 0.39017813656307D-01
2 0.58504437152421D-01 86.646 0.38958395962770D-01
3 0.97408398441585D-01 84.410 0.38839651059052D-01
.
.
.

39 0.99764986439824D+00 3.929 0.26635335895156D-02
40 0.99955382265163D+00 1.712 0.11449500031887D-02
41 0.10000000000000D+01 0.000 0.00000000000000D+00
```

This modification has no impact on the calculation of the phase functions of hydrosols and aerosols.

Change 15: Warnings removed during compilation

Need :

Some warnings can appear during the compilation. Although they do not indicate any anomalies in the implementation, this can be annoying for the user.

Evolution:

All warnings can be easily hidden using the -w option in the compilation procedure:

CCOPTS = -O3 -march=native -w.

In addition, some changes in the implementation have been made to reduce the number of potential warnings:

- In file OSOAA_MIE.F, the loop in subroutine SOS_XERO is updated:

Previous implementation	Updated implementation
DO 1 I=N,M 1 IT(I)=0.D+00	DO I=N,M IT(I)=0.D+00 ENDDO

- In file OSOAA_SURF_MATRICES.F:
 - the following loop in subroutine OSOAA_MAT_INTERFACE is updated:

Previous implementation	Updated implementation
DO 246 IJ=LIM+1,OS_NM 246 G(IJ)=0.	DO IJ=LIM+1,OS_NM G(IJ)=0. ENDDO

- In subroutine SOS_NOYAUX_FRESNEL: shared DO termination label 32, solved by adding a label 321

Previous implementation	Updated implementation
<pre>C* Boucles sur les directions Tetat et Teta2 C----- DO 32 K=1,2 J=3-K C* Initialisation des tableaux BP(IS,K)=0. ARR(IS,K)=0. ATT(IS,K)=0. GR(IS,K)=0. GT(IS,K)=0. ART(IS,K)=0 C* Boucle de sommation sur L = IS a OS_NS C----- DO 32 L=IS,OS_NS BP(IS,K)=BP(IS,K)+BETA(L)*PSL(L,J)*PSL(L,K) GR(IS,K)=GR(IS,K)+GAMMA(L)*PSL(L,J)*RSL(L,K) GT(IS,K)=GT(IS,K)+GAMMA(L)*PSL(L,J)*TSL(L,K) ATT(IS,K)=ATT(IS,K)+ALPHA(L)*TSL(L,J)*TSL(L,K)+ & ZETA(L)*RSL(L,J)*RSL(L,K) ARR(IS,K)=ARR(IS,K)+ZETA(L)*TSL(L,J)*TSL(L,K)+ & ALPHA(L)*RSL(L,J)*RSL(L,K) ART(IS,K)=ART(IS,K)+ALPHA(L)*RSL(L,K)*TSL(L,J)+ & ZETA(L)*RSL(L,J)*TSL(L,K) 32 CONTINUE ! boucle sur K et L</pre>	<pre>C* Boucles sur les directions Tetat et Teta2 C----- DO 32 K=1,2 J=3-K C* Initialisation des tableaux BP(IS,K)=0. ARR(IS,K)=0. ATT(IS,K)=0. GR(IS,K)=0. GT(IS,K)=0. ART(IS,K)=0 C* Boucle de sommation sur L = IS a OS_NS C----- DO 321 L=IS,OS_NS BP(IS,K)=BP(IS,K)+BETA(L)*PSL(L,J)*PSL(L,K) GR(IS,K)=GR(IS,K)+GAMMA(L)*PSL(L,J)*RSL(L,K) GT(IS,K)=GT(IS,K)+GAMMA(L)*PSL(L,J)*TSL(L,K) ATT(IS,K)=ATT(IS,K)+ALPHA(L)*TSL(L,J)*TSL(L,K)+ & ZETA(L)*RSL(L,J)*RSL(L,K) ARR(IS,K)=ARR(IS,K)+ZETA(L)*TSL(L,J)*TSL(L,K)+ & ALPHA(L)*RSL(L,J)*RSL(L,K) ART(IS,K)=ART(IS,K)+ALPHA(L)*RSL(L,K)*TSL(L,J)+ & ZETA(L)*RSL(L,J)*TSL(L,K) 321 CONTINUE !boucle sur L 32 CONTINUE ! boucle sur K et J</pre>

- In file OSOAA_SOS_CORE.F:
 - In subroutine OSOAA_NOYAUX : shared DO termination label 32, solved by adding a label 321
 - In subroutine OSOAA_FSOURCE_ATM_ORDREIG:
 - shared DO termination label 455, solved by adding a label 466
 - shared DO termination label 45, solved by adding a label 46
 - In subroutine OSOAA_FSOURCE_SEA_ORDRE1_MERPLATE:
 - shared DO termination label 455, solved by adding a label 466
 - shared DO termination label 45, solved by adding a label 46
 - In subroutine OSOAA_FSOURCE_SEA_ORDREIG:
 - shared DO termination label 455, solved by adding a label 466
 - shared DO termination label 45, solved by adding a label 46
 - In subroutine OSOAA_INTEGR_EPOPT_ATM_UP:
 - shared DO termination label 108, solved by adding a label 109
 - In subroutine OSOAA_INTEGR_EPOPT_ATM_DOWN:
 - shared DO termination label 109, solved by adding a label 110
 - In subroutine OSOAA_INTEGR_EPOPT_SEA_UP:
 - shared DO termination label 108, solved by adding a label 109
 - In subroutine OSOAA_INTEGR_EPOPT_SEA_DOWN:
 - shared DO termination label 109, solved by adding a label 110
 - In subroutine OSOAA_FSOURCE_DIFF_FRESNEL1:
 - shared DO termination label 10, solved by adding a label 11

Finally, blank characters at the end of instruction lines have been removed to prevent the 'Line truncated' warning message from appearing.

It has been verified that these modifications have absolutely no impact on the simulation results.

Change 16: Avoid conflicts when running several OSOAAs simultaneously

Need :

The result directory is defined by the user in the OSOAA script. If it has already been generated, a check of the content of the result directory allows estimating if the simulation is a re-run with the same geo-physical parameters, but for a different output level or a different viewing direction. The check is based on the content of the file 'ListParam.txt' file located in the result directory. A copy of this file is created in the OSOAA/exe directory, then its content is compared to the current simulation parameters. In the case of multiple OSOAA runs simultaneously, there may be a potential conflict in the comparison as the copy of the 'ListParam.txt' file can be overwritten by another run.

The same potential conflict exists during several simultaneous runs with the comparison of the 'config.txt' files (containing all the dimension parameters and the default parameters), located in the results directory and in the OSOAA/exe directory.

Evolution:

To make feasible multiple OSOAA runs simultaneously without conflicts:

- The 'copy_ListParam.txt' file is now written in the result directory rather than in the current OSOAA/exe folder.
- The output of the comparison of the 'config.txt' files, which are in the result folder and in the current OSOAA/exe directory, is now written to the result directory rather than the current OSOAA/exe folder.

These changes are made in the OSOAA_MAIN.F file.

Change 17: Degree of polarization (DoLP) control

Need :

When the radiance field becomes very small (I, Q, U), the computation of the degree of polarization (DoLP) may lead to a value higher than 100% due to machine rounding issues.

Evolution:

The degree of polarization is now controlled in the subroutine OSOAA_POLAR, in the OSOAA_SOS.F file: If its value is higher than 100%, then its value is changed to the undefined value (UNDEFINED_VALUE)

This value is given in OSOAA_SOS.F by: *#define UNDEFINED_VALUE -999.*

Change 18: Minimum number of sea layers

Need :

The setting of the sea depth (-SEA.Depth parameter) with a value lower than $0.5 \times \text{CTE_SEA_DEPTH_STEP}$ causes NaN in output files. The CTE_SEA_DEPTH_STEP parameter is defined in inc/OSOAA.h like the sampling step of the oceanic profile (in meter).

Evolution:

The minimum number of sea layers is now controlled, in the subroutine OSOAA_PROFILE (file OSOAA_PROFILE.F): If NZ = 0, then its value is forced to 1.

Change 19: Avoid reflectance values cut out in output files

Need :

If reflectance value or polarized reflectance value is lower than 10^{-100} , then the result written in output files is cut out.

For instance:

- if the reflectance is 1×10^{-100} , the written value is : 0.100000E-99
- if the reflectance is 0.9×10^{-100} , the written value is : 0.900000-100 (The E of the exponential notation is cut out)

Evolution:

To avoid this potential anomaly, a new subroutine called OSOAA_CALC_REFL (in OSOAA_SOS.F file) has been implemented.

This subroutine checks that the downward flux is not zero before calculating:

- The reflectance : $\rho = \frac{\pi \times I}{\text{Flux}_{\text{Down}}}$
- The polarized reflectance : $\rho_{\text{pol}} = \frac{\pi \times I_{\text{pol}}}{\text{Flux}_{\text{Down}}}$

If the downward flux is zero, the reflectance is set to UNDEFINED_VALUE (-999)

Finally,

If $\rho < 10^{-100}$ then ρ is set to zero.

If $\rho_{\text{pol}} < 10^{-100}$ then ρ_{pol} is set to zero.

Change 20: Use of the Morel's model [1974] to calculate the scattering coefficient of pure seawater

Need :

The CTE_FIC_MOL_SPECTRAL_DATA file (defined in OSOAA.h) provides both sea molecular absorption and scattering coefficients. For the wavelength of the radiance simulation (**OSOAA.Wa**) the absorption coefficient is linearly interpolated from the tabulated values.

The scattering coefficient is calculated in the same way, whereas it should be calculated according to Morel's model (1974), as indicated in the user's manual:

$$b_w(\lambda) = 0,00288 \times \left(\frac{\lambda}{500} \right)^{-4,32}$$

where λ is the wavelength of light in air (in nm)..

Evolution:

The subroutine OSOAA_SEA_MOL_COEFFS, in the OSOAA_PROFILE.F file, has been modified to calculate the scattering coefficient of pure seawater using Morel's model.

Change 20: Updates of the User Manual and Tutorial

Evolutions of the User Manual are listed in section “Document Change Record”

The tutorial is updated to show the new Graphical Unit Interface (GUI) of the OSOAA software.