OSOAA-User-Manual

Edition :	**01**	Date :	**2015/06/24**
Revision :	**01**	Date :	**2016/11/04**

OSOAA

Ocean Successive Orders with Atmosphere - Advanced

User Manual

OSOAA code version 1.4

Software distribution by Pr **Malik CHAMI** (LOV / UPMC)

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Document change record

Version	Date	Reasons for evolution
1.0	June 24^{th} , 2015	1^{st} issue
1.1	November 4^{th} , 2016	Information on the compilation test is included in §2.3.2

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1. Introduction

Authors:

This project has been supported by **CNES**.

The scientific supervision was carried out by **LOV** (Pr. Malik Chami - chami@obs-vlfr.fr).

The specifications for a roughness surface and software developments have been performed by **CS SI** company (Dr. Bruno Lafrance – bruno.lafrance@c-s.fr).

Acknowledgments: The authors are grateful to J. Chowdhary (GISS-NASA) for his precious contribution to inter-comparisons exercise between OSOAA model and his code.

1.1 Overview of OSOAA functionalities

Based on the successive orders of scattering method [Deuze et al, 1989, - DR5] [Lenoble et al., 2007 - DR9], the initial OSOA (Ocean Successive Orders with Atmosphere) code was the first version of a radiative transfer model for the computation of radiance and polarization in an ocean-atmosphere system, accounting for a flat surface [Chami et al., 2001 - DR2].

The OSOA-Advanced code (so-called OSOAA) introduces the capability to simulate a more realistic air / sea interface by taking into account the roughness of the sea surface as modelled by Cox & Munk [Cox and Munk, 1954 - DR4]. Note that OSOAA model allows the computation of the polarization state of light (it is a vector radiative transfer model). This new code also offers a user friendly interface (GUI) and simplified command lines to perform a set of simulation.

OSOAA allows simulating:

- **Atmospheric and sea profiles**:

  For the characterization of the atmosphere, the user can define the molecular and aerosol optical thickness.

  For the characterization of the water column, the chlorophyll and mineral-like particles concentrations are used as inputs of the code. The chlorophyll profile can be a homogeneous profile, a Gaussian profile or a user's one. The absorption of yellow substance and detritus (dead phytoplankton particles) is also modelled.

- **Aerosol models**:

  A wide variety of aerosol size distribution is available in OSOAA model to make the optical properties of the atmosphere highly close to real-world conditions. Log-normal (LND) or Junge mono-modal size distributions, bimodal LND, or pre-calculated WMO [WMO, 1986 - DR16] or Shettle & Fenn models [Shettle and Fenn, 1979 - DR14]) can be used.

  The user can also use its own aerosol phase function and radiative properties.

- **Hydrosol models**:

  Phytoplankton and Mineral-Like Particles, including their scattering and absorbing properties, can be simulated.

  The user can use its own hydrosol phase function and radiative properties.

- **Sea surface interface**:

  The air / sea interface could be modelled either for a flat surface or by taking into account of the sea roughness defined by the wind speed and the correlated waves [Cox and Munk, 1954 - DR4].

  OSOAA calculates the light transmission through the sea surface from air to sea and from sea to air. It calculates the upward reflection of the downwelling radiance field of the atmosphere on the surface and also the downward reflection of the upwelling radiance field below the surface.

The user can define specific angles for which output simulated radiance are required.

OSOAA provides the radiance field for a given altitude in the atmosphere or depth in the ocean. It can also provide the radiance profile for a specified direction. It is also possible to get the complete radiance field (upward and downward radiance in term of intensity and polarized radiance throughout the atmospheric and marine profiles).

1.2 Reference documents

DR1	Bricaud, A., Morel, A., Babin, M., Allali, K. and H. Claustre, « Variations of light absorption by suspended particles with the chlorophyll a concentration in oceanic (Case 1) waters : analysis and implications for bio-optical models ». *J. Geophysical Research*, vol. 103, pp. 31,033-31,044, 1998
DR2	Chami M., Santer R., and E. Dilligeard, « Radiative transfer model for the computation of radiance and polarization in an ocean-atmosphere system: polarization properties of suspended matter for remote sensing », *Applied Optics*, 40, 15, 2398-2416, 2001.
DR3	Chowdhary J., Cairns B., and L.D. Travis, "Contribution of water-leaving radiances to multiangle, multispectral polarimetric observations over the open ocean: bio-optical model results for case 1 waters," *Applied Optics*, Vol. 45, n°22, 5542-5567, 2006
DR4	Cox C. and W. H. Munk, « Measurements of the Roughness of the Sea Surface from Photographs of the Sun's Glitter », *J. Optical Soc. America*, Vol. 44, No. 11, 1954.
DR5	Deuzé J.L, M. Herman, and R. Santer, « Fourier series expansion of the transfer equation in the atmosphere-ocean system », *J. Quant. Spectrosc. Radiat. Transfer*, vol. 41, no. 6, pp. 483-494, 1989.
DR6	Dubovik, O.et al., « Application of spheroid models to account for aerosol particle nonsphericity in remote sensing of desert dust », *J. Geophys. Res.*, 111, D11208, doi:10.1029/2005JD006619, 2006.
DR7	Hansen J. and Travis L., "Light scattering in planetary atmospheres", *Space Sci. Rev.*, Vol. 16., pp. 527-610, 1974.

DR8	Kou, L., D. Labrie, P. Chylek, "Refractive indices of water and ice in the 0.65-2.5 m spectral range,", *Applied Optics*, 32, 3531-354, 1993
DR9	Lenoble J., M. Herman, J.L. Deuzé, B. Lafrance, R. Santer, D. Tanré, « A successive order or scattering code for solving the vector equation of transfer in the earth's atmosphere with aerosols », *J. Quant. Spectrosc. Radiat. Transfer*, vol. 107, pp. 479-507, 2007.
DR10	Mie G., Beiträge zur Optik trüber Medien, speziell kolloidaler Metallösungen, *Annalen der Physik*, vol. 330, Issue 3, pp.377-445, 1908.
DR11	Morel, A.: « Optical properties of pure water and pure sea water »,. Chapter 1 in *Optical Aspects of Oceanography*, edited by N.G. Jerlov and E.S. Nielsen, Academic Press, New-York, pp. 1-24, 1974.
DR12	Morel, A., « Optical modeling of the upper ocean in relation to its biogenous matter content (case 1 water) », *J. Geophys. Res*, vol. 93 (C9), pp. 10749-10768, 1988.
DR13	Pope, R. M., and E. S. Fry, « Absorption spectrum (380-700 nm) of pure water. II. Integrating cavity measurements », *Appl. Opt.*, vol. 36, pp. 8710-8723, 1997.
DR14	Shettle Eric P. and Fenn Robert W., « Models for the Aerosols of the Lower Atmosphere and the Effects of Humidity Variations on Their Optical Properties », Air Force Geophysics Laboratory. September 1979, AFGL-TR-79-0214, *Environnemental Research papers*, No. 676.
DR15	Smith, R.C. & K. S. Baker, « Optical properties of the clearest natural waters », *Appl. Opt.*, vol. 20, pp. 177-184, 1981.
DR16	World Climate Research Programme, « A preliminary cloudless standard atmosphere for radiation computation », *WCP-112, WMO/TD Report No 24*, Geneva, Switzerland, March 1986

1.3 Glossary

The acronyms used in this document are listed below.

AOT	Aerosol optical thickness
BRDF	Bidirectional Reflectance Distribution Function
BPDF	Bidirectional Polarization Distribution Function
CDOM	Color Dissolved Organic Matter
CNES	Centre National d'Etudes Spatiales
CS SI	Communication & Systems – Information Systems
GUI	Graphical User Interface
LND	Log Normal Distribution
LOA	Laboratoire d'Optique Atmosphérique
LOV	Laboratoire d'Océanographie de Villefranche-Sur-Mer
OSOA	Ocean Successive Orders with Atmosphere

OSOAA	Ocean Successive Orders with Atmosphere - Advanced
SOS	Successive Orders of Scattering
TOA	Top Of Atmosphere
UPMC	Université Pierre et Marie Curie

2. Software installation

2.1 Software and hardware environment

The OSOAA code runs on the following platforms:

✓ SUN machine mounted with SOLARIS operating system,

✓ PC mounted with RedHat or Ubuntu Linux

Using a **fortran 77** compiler (f77, g77 or gfortran).

Note: the application provides output binary files (radiative properties of particles from Mie calculations and surface reflection or transmission matrices computations) for which the formats are not compatible between Solaris and Linux architectures (data are recorded with different endianness: Most Significant Bit First against Least Significant Bit First). Therefore, it is not possible to use on a Solaris architecture a database generated on a Linux architecture (or reciprocally).

2.2 OSOAA deliverable contents

The OSOAA arborescence must be installed on the user account.

The file structure is composed of the following sub-directories:

- **src**: contains the code sources

OSOAA_MAIN.F	Main program of OSOAA. Manages the simulation parameters and the software run.
OSOAA_ANGLES.F	Manages angles and expansion orders.
OSOAA_AEROSOLS.F	Computes aerosol radiative properties.
OSOAA_HYDROSOLS.F	Computes hydrosol radiative properties.
OSOAA_MIE.F	Computes MIE calculation of radiative properties as a function of the size parameter.
OSOAA_PARTICLES_RAD.F	Contains routines used to compute the radiative properties of particles (aerosols and hydrosols).
OSOAA_PROFILE.F	Defines the atmospheric and maritime optical thickness profiles.
OSOAA_SURFACE.F	Manages the calculation of surface reflection and transmission BRDF / BPDF matrices.

OSOAA_SURF_MATRICES.F	Contains routines used to compute the surface reflection and transmission matrices.
OSOAA_SOS.F	Manages the radiative transfer simulation from the radiative properties of particles (aerosols and hydrosols), the optical thickness profiles (atmosphere and sea) and the sea/atmosphere interface matrices. Manages the generation of output files.
OSOAA_SOS_CORE.F	Computes the Successive Orders calculations as a function of the viewing angle, for a Fourier series expansion on the azimuth.
OSOAA_TRPHI.F	Computes the final radiance field as a function of the viewing angle and azimuth, from Fourier series expansion.

- **obj**: folder for compiled files

- **exe**: contains the executable code and initial launch scripts

- **ihm**: contains the Graphical User Interface tools

- **inc**: contains the file OSOAA.h which lists all the constant parameters (see section 3.1) shared by the different programs. It specifies the names of predefined physical data files (WMO and Shettle & Fenn aerosol models, euphotic depth depending on chlorophyll concentration, sea molecules absorption and scattering coefficients, coefficients used for calculation of phytoplankton absorption). OSOAA.h provides default values of physical parameters and of inner array size dimensions. This file also defines a set of thresholds used for computations.

- **gen**: contains the Makefiles used for the compilation

- **fic**: contains data files required for the processing:
    - Aerosol data files issued from WMO and Shettle & Fenn models: *DataWMO*, *DataSF*, *IRefrac_LR*, *IRefrac_LU*, *IRefrac_OM*, *IRefrac_SR*, *IRefrac_SU*.
    - Spectral information on scattering and absorption coefficients of sea molecules and phytoplankton: *OSAA_SEA_MOL_COEFFS.txt*, *OSAA_SEA_PHYT_COEFFS.txt*.
    - Information on the euphotic depth as a function of the surface chlorophyll concentration: *OSAA_SEA_EUPH_DEPTH.txt*.

- **doc**: contains the documentation

2.3 Compiling

2.3.1 Environment variable definition

The user must define the ***environment variable*** ***OSOAA_ROOT*** which points on the OSOAA main folder path.

It is recommended to define the variable OSOAA_ROOT in a configuration file of the user account (".profile", ".kshrc" or ".cshrc" for instance).

Example on a SOLARIS machine (KornShell):

> export OSOAA_ROOT /users/username/OSOAA_V1.0

> ls $OSOAA_ROOT must display all sub-directories listed in section 2.2.

Example on a PC linux machine within a file ".cshrc" :

setenv OSOAA_ROOT /home/usersname/OSOAA_V1.0/

2.3.2 Performing the compilation

Let's change the current directory to gen (> **cd $OSOAA_ROOT/gen**) and run the makefile:

> **make –f Makefile_OSOAA.xxx**

with xxx=**g77**, **f77** or **gfortran** depending on the available compiler

Upon completion, one can find:

> **ls $OSOAA_ROOT/obj**: object files produced by the compiler

> **ls $OSOAA_ROOT/exe**: the executable code ***OSOAA_MAIN.exe*** in addition to the initial launch scripts located in this directory.

Note: if the program has to be re-compiled, the object files located in the **$OSOAA_ROOT/obj** directory should be first removed prior to run the makefile.

The compilation was successfully tested for following configurations:

	Compiler version	**System**
f77	f90: Sun Fortran 95 8.3 SunOS_sparc 2007/05/03	Sun Solaris computer SUNW, Sun-Fire-V240; sparc; sun4u
g77		
gfortran	gcc version 4.4.7 20120313 (Red Hat 4.4.7-4) (GCC)	x86_64-redhat-linux

3. Operating mode

This chapter describes the procedure to use to execute a simulation with OSOAA code.

The processing parameters are divided into two set of parameters:

- ✓ Dimensioning parameters, predefined physical parameters and threshold values assigned in the include file **OSOAA.h**. (**$OSOAA_ROOT/inc/)**
- ✓ Physical parameters specific to the simulation, specified in the **runOSOAA**.ksh file (or .csh) (**$OSOAA_ROOT/exe/)** <u>or</u> specified with the **GUI ($OSOAA_ROOT/ihm)**.

3.1 Constants

All constants of the code are defined in the **OSOAA.h** file, located in the sub-directory ***inc*** (**$OSOAA_ROOT/inc/).**

These constants are taken into account during the compilation phase.

The change of a constant parameter in OSOAA.h **will only be effective after the re-compilation of the OSOAA software**

The OSOAA.h file specifies 6 types of constant parameters:

- ✓ Constant values common to all programs such as length of character arrays.
- ✓ Constant values specific to the computation of particles radiative properties.
- ✓ Constant values specific to computation of surface interface matrices.
- ✓ Constant values specific to the radiative transfer equation calculation, including threshold values in particular for testing whether the end of the processing has been reached.
- ✓ Constant values specific to angle definition and orders for the Fourier series and Legendre polynomials expansions.
- ✓ Constant values specific to atmospheric and maritime profiles definition.

A modification of the include file OSOAA.h is unusual. **Any change to its content requires a significant expertise and an in-depth knowledge of the analytical solution of the radiative transfer equation.**

Table 1 : list of the various constants that are mentioned in the OSOAA.h file

Constant	Default value
Common constants: Length of character chains	
Length of directory name **CTE_LENDIR**	350
Length of filename (without the directory tree) **CTE_LENFIC1**	150
Length of complete filename (with the complete directory tree) **CTE_LENFIC2**	450
Maximum size of the Keywords for the user's parameters definition **CTE_LENKEYWORD**	30
Length of command system chains **CTE_LENCOM**	400
Common constants: ID for values not defined by the user	
Allocated value for parameters of integer type, not defined by the user. **CTE_NOT_DEFINED_VALUE_INT**	-999
Allocated value for parameters of double precision type, not defined by the user. **CTE_NOT_DEFINED_VALUE_DBLE**	-999.D+00
Specific constants related to the computation of particles radiative properties	
Default filename for the aerosols radiative properties definition **CTE_DEFAULT_FICGRANU_AER**	"PM_AER.txt"
Default filename for the phytoplankton radiative properties definition **CTE_DEFAULT_FICGRANU_PHYTO**	"PM_PHYTO.txt"
Default filename for the Mineral-Like Particles radiative properties definition **CTE_DEFAULT_FICGRANU_MLP**	"PM_MLP.txt"
Size of Mie arrays as a function of the size parameter **CTE_MIE_DIM**	10000
Maximal size of user phase function arrays (for the use of external data provided by the user) **CTE_MAXNB_ANG_EXT**	200
Default value for the maximum radius of aerosols particles for a Junge model of size distribution (used if the user does not define himself the value) **CTE_DEFAULT_AER_JUNGE_RMAX**	50.

Constant	Default value
Default value for the minimum radius of hydrosols particles for a Junge model of size distribution (used if the user does not define himself the value)	
CTE_DEFAULT_HYD_JUNGE_RMIN	0.01
Default value for the maximum radius of hydrosols particles for a Junge model of size distribution (used if the user does not define himself the value)	
CTE_DEFAULT_HYD_JUNGE_RMAX	200.
Corrective value for the slope of Junge model in the case of the user has defined the singular value slope = 3 (which is not theoretically correct)	
CTE_JUNGE_SLOPE_COR	0.05
Limit value of the size parameter to calculate the MIE files for WMO and Shettle & Fenn model particles	
CTE_ALPHAMAX_WMO_DL	4000.
CTE_ALPHAMAX_WMO_WS	50.
CTE_ALPHAMAX_WMO_OC	800.
CTE_ALPHAMAX_WMO_SO	10.
CTE_ALPHAMAX_SF_SR	70.
CTE_ALPHAMAX_SF_SU	90.
Minimal value of the size distribution ratio n(r) / Nmax used to estimate the limit value of the size parameter required for Mie calculations.	
CTE_COEF_NRMAX	0.002
File containing information on WMO particle models: modal radius, log of standard deviation, volumic concentration and refractive index values (real and imaginary parts) as a function of the wavelength.	
CTE_AER_DATAWMO	"Data_WMO"
File containing information on Shettle & Fenn particle size distributions: log of standard deviation and modal radius values as a function of the relative humidity.	
CTE_AER_DATASF	"Data_SF"
Files containing information on the refractive index of Shettle & Fenn particles (real and imaginary parts) as a function of the wavelength and relative humidity.	
CTE_AER_SR_SF	"IRefrac_SR"
CTE_AER_LR_SF	"IRefrac_LR"
CTE_AER_SU_SF	"IRefrac_SU"
CTE_AER_LU_SF	"IRefrac_LU"
CTE_AER_OM_SF	"IRefrac_OM"

Constant	Default value
Angles (cosine of angles) used to define the angular range for the phase function linearization while applying a truncation.	
CTE_AER_MU1_TRONCA	0.8
CTE_AER_MU2_TRONCA	0.94
CTE_HYD_MU1_TRONCA	0.85
CTE_HYD_MU2_TRONCA	0.92
Truncation threshold: the phase function truncation is cancelled if the truncation coefficient is lower than this threshold.	
CTE_PH_SEUIL_TRONCA	0.1
Specific constants related to the computation of surface interface matrixes	
Threshold on maximal value of wave probability GMAX	
CTE_THRESHOLD_GMAX	1.D-40
Dichotomy threshold on incidence angle calculation	
CTE_THRESHOLD_DICHO	1.D-10
Threshold on minimal value for the cosine of zenith angle of the vector perpendicular to the facet of the wave estimated to an air -> sea coupled directions (incidence, transmission).	
CTE_THRESHOLD_COSTHETAN	0.001
Threshold for the dichotomic estimation of possible geometric configurations in case of transmission	
CTE_THRESHOLD_GEO_CONFIG	1.D-15
Factor used to compare GMIN and GMAX (probability function of waves)	
CTE_PH_TEST	10000
Number of azimuthal angles (= 2CTE_PH_NQ) for the calculation of the wave probability function for a given couple of incidence zenith angle and deviated zenith angles	
CTE_PH_NU	1024
Value of the exponent CTE_PH_NQ giving CTE_PH_NU = (2)CTE_PH_NQ	
CTE_PH_NQ	10
Value of the threshold for maximal order estimate of the Fourier expansion of the wave probability function	
CTE_THRESHOLD_G_SMAX	0.0001
Specific constants related to the radiative transfer equation calculation	
Default filename for the binary result file of radiance in Fourier series expansion	
CTE_DEFAULT_FICSOS_RES_BIN	"LUM_SF.bin"
Default filename for the radiance result file as a function of the zenith angle	
CTE_DEFAULT_FICSOS_RES_VS_VZA	"LUM_vsVZA.txt"

Constant	Default value
Default value of the maximal number of interaction (scattering, reflection)	
CTE_DEFAULT_IGMAX	100
Minimal wavelength for radiance calculation (µm)	
CTE_WAMIN	0.299
Factor of molecular depolarization in the air	
CTE_MDF_AIR	0.0279
Factor of molecular depolarization in the sea water	
CTE_MDF_SEA	0.0906
Threshold to test the convergence of geometric series	
CTE_PH_SEUIL_CV_SG	0.005
Threshold to test the stop of cumulative scatterings	
CTE_PH_SEUIL_SUMDIF	0.001
Threshold to test the stop of Fourier series expansion	
CTE_PH_SEUIL_SF	0.0002
Thresholds to calculate the rotation angles between scattering planes and meridian planes	
CTE_SEUIL_Z	0.0001
CTE_SEUIL_EPSILON	0.00001
Threshold value under which Q or U is fixed to be null	
CTE_THRESHOLD_Q_U_NULL	1.D-10
Value of the solar disc solid angle (sr) for the mean Earth-Sun distance	
CTE_SOLAR_DISC_SOLID_ANGLE	6.8D-5
Specific constants related to the definition of angles and orders of Legendre series expansion	
Constants related to the size of the tables of angles and limit order of Fourier series expansion.	
Maximum number of angles (positive value) used to define the size of phase functions tables. Advices: * Must be at least the default value CTE_DEFAULT_NBMU_MIE + the maximum number of user's angles CTE_NBMAX_USER_ANGLES * Must be adjusted if the common use requires more Gauss' angles than the default value. * But, do not define a too high value in order to avoid reducing the calculation velocity.	
CTE_MIE_NBMU_MAX	510

<table>
<tr><th>Constant</th><th>Default value</th></tr>
<tr><td colspan="2">Maximum number of angles (positive value) used to define the size of radiance and interface matrix tables.
Advices:
* Must be at least the default value CTE_DEFAULT_NBMU_LUM + the maximum number of user's angles CTE_NBMAX_USER_ANGLES
* Must be adjusted if the common use requires more Gauss' angles than the default value.
* But, do not define a too high value in order to avoid reducing the calculation velocity.</td></tr>
<tr><td>CTE_OS_NBMU_MAX</td><td>510</td></tr>
<tr><td colspan="2">Maximum order of Fourier series expansion and limit order for the Legendre polynomial expansion to define the size of tables used by the code.
Advice: let's define CTE_OS_NB_MAX >= 2×CTE_MIE_NBMU_MAX</td></tr>
<tr><td>CTE_OS_NB_MAX</td><td>1024</td></tr>
<tr><td colspan="2">Maximum order of Legendre polynomial expansion to define the size of tables used to compute the Fresnel matrix elements.
Advice: let's define CTE_OS_NS_MAX = 2×CTE_OS_NBMU_MAX</td></tr>
<tr><td>CTE_OS_NS_MAX</td><td>1024</td></tr>
<tr><td colspan="2">Maximum order of Fourier series expansion to define the size of tables used to compute the G function (statistic of wave slopes).
Advice: let's define CTE_OS_NM_MAX = CTE_OS_NB_MAX + CTE_OS_NS_MAX</td></tr>
<tr><td>CTE_OS_NM_MAX</td><td>2048</td></tr>
<tr><td colspan="2">Default number of angles and maximum orders of series expansions to be used in the case of none definition of angles by the user</td></tr>
<tr><td colspan="2">Default number of Gauss' angles (positive values) to be used for the Mie phase function calculations</td></tr>
<tr><td>CTE_DEFAULT_NBMU_MIE</td><td>40</td></tr>
<tr><td colspan="2">Default number of Gauss' angles (positive values) to be used for the radiance calculations</td></tr>
<tr><td>CTE_DEFAULT_NBMU_LUM</td><td>48</td></tr>
<tr><td colspan="2">Default value for the limit order of Legendre polynomial and Fourier series expansion to compute radiance :
Usually : CTE_DEFAULT_OS_NB = 2×CTE_DEFAULT_NBMU_MIE</td></tr>
<tr><td>CTE_DEFAULT_OS_NB</td><td>80</td></tr>
<tr><td colspan="2">Default value for the limit order of Legendre polynomial expansion to compute the Fresnel matrix elements
Usually : CTE_DEFAULT_OS_NS = 2×CTE_DEFAULT_NBMU_LUM</td></tr>
<tr><td>CTE_DEFAULT_OS_NS</td><td>96</td></tr>
<tr><td colspan="2">Default value for the limit order of Fourier series expansion of the G function (statistic of wave slopes).
It is necessary than
CTE_DEFAULT_OS_NM >= CTE_DEFAULT_OS_NB + CTE_DEFAULT_OS_NS</td></tr>
<tr><td>CTE_DEFAULT_OS_NM</td><td>176</td></tr>
</table>

Constant	Default value
Limitation of the number of angles in order to define the angles set to be used for simulations	
Maximum number of user's angles to be added to the Gauss angles	
CTE_NBMAX_USER_ANGLES	40
Maximum number of positive angles for the calculation of angles to be used by the routines (Gauss angles + user's angles + 1 = solar zenith angle) Advice : it should be the max between CTE_MIE_NBMU_MAX and CTE_OS_NBMU_MAX	
CTE_NBANGLES_MAX	1000
Minimum absolute difference between cos(X) and cos(θ) to assign θ = X	
CTE_SEUIL_ECART_MU	0.00001
Default name of result angles files	
Default filename for the definition of angles and orders of Legendre series expansion applied to the radiance calculations	
CTE_DEFAULT_FICANGLES_RES_LUM	"RAD_UsedAngles.txt"
Default filename for the definition of angles and orders of Legendre series expansion applied to the Mie calculations	
CTE_DEFAULT_FICANGLES_RES_MIE	"MIE_UsedAngles.txt"
Specific constants related to the calculation of atmospheric and maritime profiles	
Default filename for the definition of the atmospheric profile	
CTE_DEFAULT_FICPROFIL_ATM_RES	"PROFILE_ATM.txt"
Default filename for the definition of the sea profile	
CTE_DEFAULT_FICPROFIL_SEA_RES	"PROFILE_SEA.txt"
Standard Pressure (mb)	
CTE_STD_PRESSURE	1013
Altitude of the Top of Atmosphere (km)	
CTE_ALT_TOA	300.
Number of atmospheric layers	
CTE_NT_ATM	26
Number of sea layers	
CTE_NT_SEA	80
Optical thickness of the transition layer atmosphere / sea	
CTE_TRANS_OPT_THICKNESS	0.0001
Maximum number of layers used to profile computations	
CTE_NZ_MAX	25000
Sampling step of the oceanic profile (m)	
CTE_SEA_DEPTH_STEP	0.05

Constant	Default value
Filename of euphotic depth depending on chlorophyll concentration (Morel table) #define	
CTE_FIC_EUPH_DEPTH	"OSOAA_SEA_EUPH_DEPTH.txt"
Filename of the sea molecules absorption and scattering coefficients	
CTE_FIC_MOL_SPECTRAL_DATA	"OSOAA_SEA_MOL_COEFFS_JUNE_2013.txt"
Filename of the AP and EP coefficients to be used for the calculation of phytoplankton absorption	
CTE_FIC_PHYTO_SPECTRAL_DATA	"OSOAA_SEA_PHYT_COEFFS.txt"
Maximum number of spectral data in files defined by CTE_FIC_MOL_SPECTRAL_DATA and CTE_FIC_PHYTO_SPECTRAL_DATA	
CTE_NBWA_MAX	2500
Default value of the coefficient for the spectral variation of yellow substance absorption (m^{-1})	
CTE_DEFAULT_SPECTRAL_YS	0.01
Default value of the coefficient for the spectral variation of detritus absorption (m^{-1})	
CTE_DEFAULT_SPECTRAL_DET	0.011
Maximal value of the sea column optical thickness	
CTE_SEA_T_LIMIT	**30.**

3.2 Simulation parameters

The simulation parameters can be distinguished in 7 sets of parameters:

- ✓ General parameters: see §3.2.1.
- ✓ Atmospheric and sea profile parameters: see §3.2.2, page 23.
- ✓ Aerosols parameters: see §3.2.3, page 27.
- ✓ Hydrosols parameters (phytoplankton and sediments – also called Mineral Like-Particles): see §3.2.4, page 31.
- ✓ Sea / atmosphere interface parameters: see §3.2.5, page 37.
- ✓ Angle calculation parameters: see §3.2.6, page 37.
- ✓ Selection of expected outputs: see §3.2.7, page 39.

Each parameter is defined in a command file by a couple « **-Keyword Value** ».

The command file can be written by the user (see §3.3.1, page 42). If the *Graphical User Interface* is used to perform a simulation, then, the command file is automatically written (see §3.3.2, page 43).

The simulation parameters are listed in tables in the following sections.

A status is associated to each parameter:

- **Required (R)**: the user must define this parameter.
- **Default (D)**: the software requires a value for this parameter. If it is not defined by the user then a default value is automatically applied.

  The default value of the parameter is provided by a devoted constant value in the file OSOAA.h (located in the directory $OSOAA_ROOT/inc).
- **Optional (O)**: the definition of this parameter is optional.
- **Conditional (C)**: the definition of this parameter is required to complete the information on another parameter.

3.2.1 General parameters

The **definition of the working folder** for the OSOAA computations is ensured by the keyword **–OSOAA.ResRoot**. All the output files and log files will be located in this working folder in specific sub-directories (in the ***Advanced_Output/*** or ***Standard_Output/*** sub-directories, see 3.2.7, page 39) which are automatically created after a simulation.

The **wavelength for the radiance calculations** is defined by the keyword **–OSOAA.Wa**. Some radiative parameters must be defined for this wavelength, such as the aerosol and hydrosol refractive indices, the molecular optical thickness or surface albedos.

The **solar zenith angle** is also a specific parameter, defined by the keyword **–OSOAA.Thetas**.

The **main log file**, providing general information on the processing, is an optional output defined by the keyword **–OSOAA.Log**. The produced log file is located in the ***Advanced_Output/*** sub-directory.

Table 2 : General parameters

Parameter	Definition	R/O
-OSOAA.ResRoot	Working folder for the OSOAA computations (complete path) *String (CTE_LENDIR characters max)*	**R**
-OSOAA.Wa	Wavelength for radiance simulation (µm) *Float*	**R**
-ANG.Thetas	Solar zenith angle in degrees (0 < thetas < 90°) *Float*	**R**
-OSOAA.Log	Log filename for main computations. Only created if the log filename is specified. An already existing file will be overwritten. *String (CTE_LENFIC2 characters max)*	**O**

3.2.2 Atmospheric and sea profile parameters

The profile parameters characterize the vertical distribution of particles (hydrosols and aerosols) and the values of the reflectance/albedo of the boundary limit of the atmosphere-ocean system (i.e., sea surface foam and sea bottom albedo).

Table 3 : Parameters for the definition of the reflectance at boundary layers

Parameter	Definition	R/O
Sea surface		
SEA.SurfAlb	Sea surface albedo for the wavelength of radiance calculation (lambertian component) *Float*	**R**

Parameter	Definition	R/O
Sea bottom		
SEA.BotType	Type of sea bottom for albedo definition Cases : 1 : User's lambertian value (user data -SEA.BotAlb) 2 : Light sand (tabulated data) 3 : Green algua (tabulated data) 4 : Brown algae (tabulated data) 5 : Red algae (tabulated data) *Integer*	**R**
If SEA.BotType = 1		
SEA.BotAlb	Sea bottom albedo for the wavelength of radiance calculation (lambertian component). *Float*	**C**

Table 4 : Parameters for the atmospheric and sea profile definition

Parameter	Definition	R / O / D / C	
PROFILE.Log	Log filename for profile calculations (without directory tree) Only created if the log filename is specified. An already existing file will be overwritten. *String (CTE_LENFIC2 characters max)*	**O**	
Atmospheric profile parameter			
PROFILE_ATM.ResFile	Filename for the atmospheric profile result file (without directory tree) An already existing file will be overwritten. *String (CTE_LENFIC2 characters max)* Default value (in OSOAA.h): **CTE_DEFAULT_FICPROFIL_ATM_RES**	**D**	
Air molecules			
AP.MOT	Molecular optical thickness for the wavelength of radiance simulation *Float*	**O**	Only one of these parameters must be defined
AP.Pressure	Atmospheric pressure at sea level (mbar) *Float*	**O**	

If SEA.MOT ≥ 0.0001		
AP.HR	Height scale of the molecular profile (km). *Float*	**C**
Aerosols		
AER.Waref	Reference wavelength (µm) for the aerosol optical thickness (AER.AOTref) *Float*	**R**
AER.AOTref	Aerosol optical thickness for the reference wavelength *Float*	**R**
If AER.AOTref ≥ 0.0001		
AP.HA	Height scale of the aerosol profile (km). *Float*	**C**
Sea profile parameter		
PROFILE_SEA.ResFile	Filename for the sea profile result file (without directory tree) An already existing file will be overwritten. *String (CTE_LENFIC2 characters max)* Default value (in OSOAA.h): **CTE_DEFAULT_FICPROFIL_SEA_RES.**	**D**
Sea.Depth	Sea depth (meters) *Float* If not defined, the euphotic depth will be used from Morel tabulated data depending on the chlorophyll concentration at sea surface: **CTE_FIC_EUPH_DEPTH** file defined in OSOAA.h	**D**
Phytoplankton		
PHYTO.Chl	Chlorophyll concentration at sea surface ($mg.m^{-3}$) *Float*	**R**
If PHYTO.Chl ≥ 0		
PHYTO.ProfilType	Type of the chlorophyll profile : Cases : 1: Homogeneous profile 2: Gaussian profile 3: User's profile file *Integer*	**C1**

If PHYTO.ProfilType = 2 (Gaussian profile)		
PHYTO.GP.Chlbg	Constant biomass background (mg.m^{-3}) *Float*	**C2**
PHYTO.GP.Deep	Maximum deep of the gaussian chlorophyll profile (m) *Float*	**C2**
PHYTO.GP.Width	Peak width of the gaussian chlorophyll profile (m) *Float*	**C2**
If PHYTO.ProfilType = 3 (User profile)		
PHYTO.Userfile	Userfile describing the chlorophyll profile *String (CTE_LENFIC2 characters max)*	**C2**
Mineral-like particles		
SED.Csed	Concentration of sediment at sea surface (mg.ℓ$^{-1}$) *Float*	**R**
Yellow substance and detritus		
YS.Abs440	Absorption coefficient of yellow substance at 440 nm (m^{-1}) *Float*	**R**
If YS.Abs440 > 0.0		
YS.Swa	Coefficient for the spectral variation of the yellow substance absorption (m^{-1}) for the simulation wavelength. Default value (in OSOAA.h): **CTE_DEFAULT_SPECTRAL_YS** *Float*	**D**
DET.Abs440	Absorption coefficient of detritus at 440 nm (m^{-1}) *Float*	**R**
If DET.Abs440 > 0.0		
DET.Swa	Coefficient for the spectral variation of the detritus absorption (m^{-1}) for the simulation wavelength. Default value (in OSOAA.h): **CTE_DEFAULT_SPECTRAL_DET** *Float*	**D**

3.2.3 Aerosols parameters

The following table lists all the parameters associated to an aerosol model definition which must be defined if the aerosol optical thickness for the reference wavelength (-AER.AOTref) is not null.

Table 5 : Aerosols parameters

Parameter	Definition	O/ D/C
AER.Log	Log filename for aerosol model calculations (without directory tree) Only created if the log filename is specified. An already existing file will be overwritten. *String (CTE_LENFIC2 characters max)*	**O**
AER.MieLog	Log filename for Mie aerosol calculations (without directory tree) Only created if the log filename is specified. An already existing file will be overwritten. *String (CTE_LENFIC2 characters max)*	**O**
AER.ResFile	Filename for the aerosol radiative properties result file (without directory tree) An already existing file will be overwritten. *String (CTE_LENFIC2 characters max)* Default value (in OSOAA.h): **CTE_DEFAULT_FICGRANU_AER**	**D**
If AER.AOTref > 0.0001		
AER.DirMie	Directory for aerosol MIE files storage (complete path) *String (CTE_LENDIR characters max)*	**C1**
AER.Tronca	Option that allows to apply or not a truncation of the aerosol phase function: 0 : no truncation of the aerosol phase function 1 : a truncation of the aerosol phase function will be applied *Integer* Default value: **1**	**D**

Parameter	Definition	O/ D/C
AER.Model	Type of aerosol model 0 : Mono-modal 1 : WMO multi-modal 2 : Shettle & Fenn bi-modal 3 : Log-Normal bi-modal 4 : Phase functions from an external source *Integer*	**C1**
If AER.Model = 0 : parameters of mono-modal size distributions		
AER.MMD.MRwa	Real part of the aerosol refractive index for the wavelength of radiance calculation *Float F5.3*	**C2**
AER.MMD.MIwa	Imaginary part of the aerosol refractive index for the wavelength of radiance calculation (negative value) *Float F8.5*	**C2**
AER.MMD.SDtype	Type of mono-modal size distribution 1 : Log-Normal size distribution 2 : Junge's law *Integer*	**C2**
If AER.MMD.SDtype = 1 : Log-Normal size distribution		
AER.MMD.LNDradius	Modal radius (μm) of the Log-Normal size distribution *Float*	**C2**
AER.MMD.LNDvar	Standard deviation of the Log-Normal size distribution *Float*	**C2**
If AER.MMD.SDtype = 2 : Junge size distribution		
AER.MMD.JD.slope	Slope of the Junge's law Warning: 3 is a singular value *Float*	**C2**
AER.MMD.JD.rmin	Minimal radius of the Junge's law (μm)	**C2**
AER.MMD.JD.rmax	Maximal radius of the Junge's law (μm) *Float* Default value (in OSOAA.h): **CTE_DEFAULT_AER_JUNGE_RMAX**	**D**
If AER.Waref ≠ OSOAA.Wa		
AER.MMD.MRwaref	Real part of the aerosol refractive index for the reference wavelength of aerosol properties calculation *Float F5.3*	**C2**

Parameter	Definition	O/ D/C
AER.MMD.MIwaref	Imaginary part of the aerosol refractive index for the reference wavelength of aerosol properties calculation (negative value) *Float F8.5*	**C2**
If AER.Model = 1 : WMO aerosol model		
AER.WMO.Model	Type of WMO model. 1 : Continental WMO model. 2 : Maritime WMO model. 3 : Urban WMO model. 4 : WMO model by user definition. *Integer*	**C3**
If AER.WMO.Model = 4 : user concentrations (summation = 1)		
AER.WMO.DL	Volume concentration (between 0 and 1) of "Dust-Like" components *Float*	**C3**
AER.WMO.WS	Volume concentration (between 0 and 1) of "Water Soluble" components *Float*	**C3**
AER.WMO.OC	Volume concentration (between 0 and 1) of "OCeanic" components *Float*	**C3**
AER.WMO.SO	Volume concentration (between 0 and 1) of "SOot" components *Float*	**C3**
If AER.Model = 2 : Shettle & Fenn aerosol model		
AER.SF.Model	Shettle & Fenn model 1 : Tropospheric 2 : Urban 3 : Maritime 4 : Coastal *Integer*	**C4**
AER.SF.RH	Percentage of air relative humidity (from 0 to 99%) *Float*	**C4**
If AER.Model = 3 : Log-Normal bi-modal aerosol model		
AER.BMD.VCdef	Choice of the mixture description type 1 : Use of predefined volume concentrations 2 : Use of the ratio of aerosol optical thicknesses (coarse mode AOT / total AOT) *Integer*	**C2**

Parameter	Definition	O/ D/C
If AER.BMD.VCdef = 1 : user-defined volume concentrations		
AER.BMD.CoarseVC	User volume concentration of the "LND coarse mode" *Float*	**C3**
AER.BMD.FineVC	User volume concentration of the "LND fine mode" *Float*	**C3**
If AER.BMD.VCdef = 2 : **Use of ratio coarse mode optical thickness over total AOT**		
AER.BMD.RAOT	User value of the ration AOT_coarse / AOT_total for the aerosol reference wavelength. *Float*	**C3**
Coarse mode LND parameters		
AER.BMD.CM.MRwa	Real part of the refractive index for the "LND coarse mode" for the wavelength of radiance calculation *Float F5.3*	**C2**
AER.BMD.CM.MIwa	Imaginary part of the refractive index for the "LND coarse mode" for the wavelength of radiance calculation (negative value) *Float F8.5*	**C2**
AER.BMD.CM.SDradius	Modal radius of the "LND coarse mode" (µm) *Float*	**C2**
AER.BMD.CM.SDvar	Standard deviation of the "LND coarse mode" *Float*	**C2**
If AER.Waref ≠ OSOAA.Wa		
AER.BMD.CM.MRwaref	Real part of the refractive index for the "LND coarse mode" for the aerosol reference wavelength *Float F5.3*	**C3**
AER.BMD.CM.MIwaref	Imaginary part of the refractive index for the "LND coarse mode" for the aerosol reference wavelength (negative value) *Float F8.5*	**C3**
Fine mode LND parameters		
AER.BMD.FM.MRwa	Real part of the refractive index for the "LND fine mode" for the wavelength of radiance calculation *Float F5.3*	**C2**
AER.BMD.FM.MIwa	Imaginary part of the refractive index for the "LND fine mode" for the wavelength of radiance calculation (negative value) *Float F8.5*	**C2**

Parameter	Definition	O/ D/C
AER.BMD.FM.SDradius	Modal radius of the "LND fine mode" (µm) *Float*	**C2**
AER.BMD.FM.SDvar	Standard deviation of the "LND fine mode" *Float*	**C2**
If AER.Waref ≠ OSOAA.Wa		
AER.BMD.FM.MRwaref	Real part of the refractive index for the "LND fine mode" for the aerosol reference wavelength *Float F5.3*	**C3**
AER.BMD.FM.MIwaref	Imaginary part of the refractive index for the "LND fine mode" for the aerosol reference wavelength (negative value) *Float F8.5*	**C3**
If AER.Model = 4 : Phase functions from an external source		
AER.ExtData	Filename (complete path) of user's external phase function data and radiative parameters (extinction and scattering coefficients) Special requirement: For this specific case, the reference aerosol wavelength (-AER.Waref) and the radiance simulation wavelength (-OSOAA.Wa) must be equal. *String (CTE_LENFIC2 characters max)*	**C2**

3.2.4 Hydrosols parameters: Phytoplankton and Mineral-Like Particles

The following table lists all the parameters associated to the model definition of phytoplankton and Mineral-Like Particles. These models must be defined if the surface concentrations of these hydrosols are not null.

Table 6 : Hydrosols parameters

Parameter	Definition	O/ D/C
HYD.Log	Log filename for hydrosol models calculations (without directory tree) Only created if the log filename is specified. An already existing file will be overwritten. *String (CTE_LENFIC2 characters max)*	**O**

Parameter	Definition	O/ D/C
HYD.MieLog	Log filename for Mie hydrosol calculations (without directory tree) Only created if the log filename is specified. An already existing file will be overwritten. *String (CTE_LENFIC2 characters max)*	**O**
PHYTO.ResFile	Filename for the phytoplankton radiative properties result file (without directory tree) An already existing file will be overwritten. NB: In case of an user file is used (-HYD.ExtData), this output file contains the global coefficients of the phase function expansion in Legendre functions. *String (CTE_LENFIC2 characters max)* Default value (in OSOAA.h): **CTE_DEFAULT_FICGRANU_PHYTO**	**D**
MLP.ResFile	Filename for the Mineral-Like Particles radiative properties result file (without directory tree) An already existing file will be overwritten. NB: In case of an user file is used (-HYD.ExtData), this output file contains null coefficients for the phase matrix expansion in Legendre functions. *String (CTE_LENFIC2 characters max)* Default value (in OSOAA.h): **CTE_DEFAULT_FICGRANU_MLP**	**D**
If PHYTO.Chl > 0.0 or SED.Csed > 0.0		
HYD.DirMie	Directory for hydrosol MIE files storage (complete path) *String (CTE_LENDIR characters max)*	**C1**
HYD.Model	Type of hydrosol characterization 1: From size distribution models 2: Use of an external phase function *Integer*	**C1**
If HYD.Model = 1 : Hydrosols characterization by models		
Main mode of phytoplankton :	**Junge distribution**	
PHYTO.JD.MRwa	Real part of the refractive index for phytoplankton particles at the simulation wavelength: main mode of particles (Junge distribution). *Float F5.3*	**C2**

Parameter	Definition	O/ D/C
PHYTO.JD.MIwa	Imaginary part of the refractive index (negative value) for phytoplankton particles at the simulation wavelength: main mode of particles (Junge distribution). *Float F8.5*	**C2**
PHYTO.JD.slope	Slope of Junge's law for phytoplankton particles *Float*	**C2**
PHYTO.JD.rmin	Minimal radius of Junge's law for phytoplankton particles (µm) *Float* Default value (in OSOAA.h): **CTE_DEFAULT_HYD_JUNGE_RMIN**	**D**
PHYTO.JD.rmax	Maximal radius of Junge's law for phytoplankton particles (µm) *Float* Default value (in OSOAA.h): **CTE_DEFAULT_HYD_JUNGE_RMAX**	**D**
PHYTO.JD.rate	Ratio of the main mode in the global distribution for phytoplankton particles (as a proportion of the Junge distribution particles versus the global amount of phytoplankton particles: value between 0 and 1) *Float*	**C2**
Secondary mode of phytoplankton : LND distribution Optional parameters but the definition of one PHYTO.LND.SM.* parameter requires the definition of all the others.		
PHYTO.LND.SM.MRwa	Real part of the refractive index for phytoplankton particles at the simulation wavelength: secondary mode of particles (LND distribution). *Float F5.3*	**O**
PHYTO.LND.SM.MIwa	Imaginary part of the refractive index (negative value) for phytoplankton particles at the simulation wavelength: secondary mode of particles (LND distribution). *Float F8.5*	**O**
PHYTO.LND.SM. SDradius	Modal radius of the LND for the secondary mode of phytoplankton particles (µm) *Float*	**O**

Parameter	Definition	O/ D/C
PHYTO.LND.SM.SDvar	Standard deviation of the LND for the secondary mode of phytoplankton particles *Float*	**O**
PHYTO.LND.SM.rate	Ratio of the LND secondary mode in the global distribution for phytoplankton particles (as a proportion of the number of the secondary LND mode particles versus the global amount of phytoplankton particles) *Float*	**O**
Tertiary mode of phytoplankton : LND distribution Optional parameters but the definition of one PHYTO.LND.TM.* parameter requires the definition of all the others.		
PHYTO.LND.TM. MRwa	Real part of the refractive index for phytoplankton particles at the simulation wavelength: tertiary mode of particles (LND distribution). *Float F5.3*	**O**
PHYTO.LND.TM.MIwa	Imaginary part of the refractive index (negative value) for phytoplankton particles at the simulation wavelength: tertiary mode of particles (LND distribution). *Float F8.5*	**O**
PHYTO.LND.TM. SDradius	Modal radius of the LND for the tertiary mode of phytoplankton particles (µm) *Float*	**O**
PHYTO.LND.TM.SDvar	Standard deviation of the LND for the tertiary mode of phytoplankton particles *Float*	**O**
PHYTO.LND.TM.rate	Ratio of the LND tertiary mode in the global distribution for phytoplankton particles (as a proportion of the number of the tertiary LND mode particles versus the global amount of phytoplankton particles) *Float*	**O**
If SED.Csed > 0.0		
Main mode of Mineral-Like Particles : Junge distribution		
SED.JD.MRwa	Real part of the refractive index for mineral-like particles at the simulation wavelength: main mode of particles (Junge distribution). *Float F5.3*	**C2**

Parameter	Definition	O/ D/C
SED.JD.MIwa	Imaginary part of the refractive index (negative value) for mineral-like particles at the simulation wavelength: main mode of particles (Junge distribution). *Float F8.5*	**C2**
SED.JD.slope	Slope of Junge's law for mineral-like particles *Float*	**C2**
SED.JD.rmin	Minimal radius of Junge's law for mineral-like particles (µm) *Float* Default value (in OSOAA.h): **CTE_DEFAULT_HYD_JUNGE_RMIN**	**D**
SED.JD.rmax	Maximal radius of Junge's law for mineral-like particles (µm) *Float* Default value (in OSOAA.h): **CTE_DEFAULT_HYD_JUNGE_RMAX**	**D**
SED.JD.rate	Ratio of the main mode in the global distribution for mineral-like particles (as a proportion of the Junge distribution particles versus the global amount of mineral-like particles: value between 0 and 1) *Float*	**C2**
Secondary mode of Mineral-Like Particles : LND distribution Optional parameters but the definition of one SED.LND.SM.* parameter requires the definition of all the others.		
SED.LND.SM.MRwa	Real part of the refractive index for mineral-like particles at the simulation wavelength: secondary mode of particles (LND distribution). *Float F5.3*	**O**
SED.LND.SM.MIwa	Imaginary part of the refractive index (negative value) for mineral-like particles at the simulation wavelength: secondary mode of particles (LND distribution). *Float F8.5*	**O**
SED.LND.SM.SDradius	Modal radius of the LND for the secondary mode of mineral-like particles (µm) *Float*	**O**

Parameter	Definition	O/ D/C
SED.LND.SM.SDvar	Standard deviation of the LND for the secondary mode of mineral-like particles *Float*	**O**
SED.LND.SM.rate	Ratio of the LND secondary mode in the global distribution for mineral-like particles (as a proportion of the number of the secondary LND mode particles versus the global amount of mineral-like particles) *Float*	**O**
Tertiary mode of Mineral-Like Particles : LND distribution Optional parameters but the definition of one SED.LND.TM.* parameter requires the definition of all the others.		
SED.LND.TM.MRwa	Real part of the refractive index for mineral-like particles at the simulation wavelength: tertiary mode of particles (LND distribution). *Float F5.3*	**O**
SED.LND.TM.MIwa	Imaginary part of the refractive index (negative value) for mineral-like particles at the simulation wavelength: tertiary mode of particles (LND distribution). *Float F8.5*	**O**
SED.LND.TM.SDradius	Modal radius of the LND for the tertiary mode of mineral-like particles (µm) *Float*	**O**
SED.LND.TM.SDvar	Standard deviation of the LND for the tertiary mode of mineral-like particles *Float*	**O**
SED.LND.TM.rate	Ratio of the LND tertiary mode in the global distribution for mineral-like particles (as a proportion of the number of the tertiary LND mode particles versus the global amount of mineral-like particles) *Float*	**O**
If HYD.Model = 2 : Hydrosols characterization by external data		
HYD.ExtData	Filename (complete path) of user's external sea particles phase function data and radiative parameters (extinction and scattering coefficients) Special requirement: For this use case, the radiative measurements must be provided at the radiance simulation wavelength (-OSOAA.Wa). *String (CTE_LENFIC2 characters max)*	**C2**

3.2.5 Sea / atmosphere interface parameters

The sea / atmosphere interface simulates the waves shape (correlated to the wind velocity by the Cox & Munk model [DR4]) and the reflection / transmission properties of wave facets (depending on the sea refractive index according to the Fresnel's law [DR2]).

Table 7 : Sea / atmosphere interface parameters

Parameter	Definition	O/R/C
SEA.Log	Log filename for SURFACE file computations. Only created if the log filename is specified. An already existing file will be overwritten. *String (CTE_LENFIC2 characters max)*	**O**
SEA.Wind	Wind velocity at sea surface (m/s) *Float F4.1*	**R**
If SEA.Wind ≠ 0 m.s^{-1}		
SEA.Dir	Directory for SURFACE files storage (complete path) *String (CTE_LENDIR characters max)*	**C1**
SEA.Ind	Surface / atmosphere refractive index (air = 1) for the simulation wavelength *Float F5.3*	**C1**

3.2.6 Angles calculation parameters

The number of Gauss' angles to be used to discriminate the radiance field (and BRDF/BPFD interface matrices) must be defined, rather by a user definition or by the use of the default number of Gauss angles proposed by OSOAA. Similarly, it is necessary to define the number of Gauss's angles to be used to calculate scattering phase functions.

These choices impact the limit orders of series expansions, calculated by the software.

The user can define the name of the angle files that OSOAA will generate or use the default filenames.

The conventions for angle definition are explained in section 3.4.1, page 52.

Table 8 : Angles calculation parameters

Parameter	Definition	R/O/D
ANG.Log	Log filename for ANGLES calculations (without directory tree) Only created if the log filename is specified. An already existing file will be overwritten. *String (CTE_LENFIC2 characters max)*	**O**
Angles for radiance computations		
ANG.Rad.NbGauss	Number of Gauss angles to be used for radiance computations *Integer* Default value (in OSOAA.h): **CTE_DEFAULT_NBMU_LUM**	**D**
ANG.Rad.UserAngFile	Filename (complete path) of the complementary list of user's angles to complete the ANG.Rad.NbGauss angles *String (CTE_LENFIC2 characters max)*	**O**
ANG.Rad.ResFile	Filename of list of angles and maximum orders of series expansions to be used for BRDF/BPDF and radiance computations (without directory tree) *String (CTE_LENFIC2 characters max)* Default value (in OSOAA.h): **CTE_DEFAULT_FICANGLES_RES_LUM**	**D**
Angles for Mie phase function computations		
ANG.Mie.NbGauss	Number of Gauss angles to be used for phase matrix computations *Integer* Default value (in OSOAA.h): **CTE_DEFAULT_NBMU_MIE**	**D**
ANG.Rad.UserAngFile	Filename (complete path) of the complementary list of user's angles to complete the ANG.Mie.NbGauss angles *String (CTE_LENFIC2 characters max)*	**O**
ANG.Rad.ResFile	Filename of list of angles and maximum orders of series expansions to be used for phase function computations (without directory tree) *String (CTE_LENFIC2 characters max)* Default value (in OSOAA.h): **CTE_DEFAULT_FICANGLES_RES_MIE**	**D**

3.2.7 Output parameters

The output parameters defined the choice of provided output data. It is necessary to define the value of the relative azimuth angle to be used to recombine the Fourier series expansion of (I, Q, U) Stokes' parameters.

The choice of output data concerns the zenith and relative azimuth angles of the viewing direction, and the selected level in the profile.

All the produced files are automatically located in this working folder in specific sub-directories (in the Advanced_Output/ or Standard_Output/ sub-directories). Therefore, the result filenames are defined without their complete path.

Table 9 : Parameters for the selection of outputs

Parameter	Definition	R/O
SOS.Log	Log filename for SOS calculations (without directory tree) Only created if the log filename is specified. An already existing file will be overwritten. *String (CTE_LENFIC2 characters max)*	**O**
Relative azimuth angle and maximal Successive Order of Scattering definition		
OSOAA.View.Phi	Relative azimuth angle (degrees) for output radiance *Float*	**R**
SOS.IGmax	Maximal order of atmospheric and sea scattering & surface reflexion/transmission *Integer* Default value (in OSOAA.h): **CTE_DEFAULT_IGMAX**	**D**
Output files		
SOS.ResFile.Bin	Filename of the output binary file from SOS computations (without directory tree), containing (I,Q,U) in term of Fourier series expansion *String (CTE_LENFIC2 characters max)* Default value (in OSOAA.h): **CTE_DEFAULT_FICSOS_RES_BIN**	**D**

Parameter	Definition	R/O
OSOAA.ResFile.vsVZA	Filename of the output ascii file given the radiance field (I,Q,U) versus the viewing zenith angle, for the given relative azimuth angle (OSOAA.View.Phi) and given altitude or depth (OSOAA.View.Level) An already existing file will be overwritten. *String (CTE_LENFIC2 characters max)* Default value (in OSOAA.h): **CTE_DEFAULT_FICSOS_RES_VS_VZA**	**D**
OSOAA.View.Level	Index for the output level definition Cases : 1 : Top of Atmosphere 2 : Sea Bottom 3 : Over sea Surface 0+ 4 : Below sea Surface 0- 5 : User's definition of altitude or depth (user data -OSOAA.View.Z) *Integer*	**R**
If OSOAA.View.Level = 5		
OSOAA.View.Z	Altitude or depth (meters) for which the radiance has to be given versus the viewing zenith angle, (for the given relative azimuth angle OSOAA.View.Phi). *Float*	**C1**
OSOAA.ResFile.Adv.Up	Filename of the output ascii file (without directory tree) resulting from SOS computations: Advanced output **upward radiance field** versus the depth (or altitude) AND versus the viewing zenith angle (for the given relative azimuth angle OSOAA.View.Phi) An already existing file will be overwritten. *String (CTE_LENFIC2 characters max)*	**O**
OSOAA.ResFile.Adv. Down	Filename of the output ascii file (without directory tree) resulting from SOS computations: Advanced output **downward radiance field** versus the depth (or altitude) AND versus the viewing zenith angle (for the given relative azimuth angle OSOAA.View.Phi) An already existing file will be overwritten. *String (CTE_LENFIC2 characters max)*	**O**

Parameter	Definition	R/O
OSOAA.ResFile.vsZ	Filename of the output ascii file given the radiance field versus the altitude or depth (for the given relative azimuth angle and given viewing zenith angle) NB: if defined, it is required to also define **-OSOAA. View.VZA** An already existing file will be overwritten. *String (CTE_LENFIC2 characters max)*	**O**
OSOAA.View.VZA	Viewing zenith angle (degrees) for which the radiance has to be given versus the altitude or depth (for the given relative azimuth angle) NB: if defined, it is required to also define **-OSOAA.ResFile.vsZ** *Float*	**O**

3.3 Simulation launch

3.3.1 How using a command file

The following command file is an example for a radiance simulation at 440 nm, with a solar zenith angle of 30°, a standard atmospheric pressure and an aerosol optical thickness of 0.2 at 550 nm for the Maritime model of Shettle&Fenn (98% of relative humidity). The chlorophyll concentration is 0.2 mg.m^{-3} and the sea depth is at 15 m with a bottom albedo of 0.3. The wind velocity is 7 m/s at sea surface. The surface foam albedo is 0.1. The user requires an output radiance field at 10 m depth in the solar principal plan but also the global upward and downward (I,Q,U) fields throughout the air and sea profiles.

The user defines the location of the results directory and the location of the database where Mie and interface matrix files must be stored by OSOAA.

In order to perform a simulation: **$OSOAA_ROOT/exe/run_OSOAA.ksh**

```
dirRESULTS=${USER_DIRECTORY}/OSOAA_RESULTS_DEMO

dirMIE_AER=${USER_DIRECTORY }/DATABASE/MIE_AER  && mkdir -p ${dirMIE_AER}
dirMIE_HYD=${USER_DIRECTORY }/DATABASE/MIE_HYD  && mkdir -p ${dirMIE_HYD}
dirSURF=${USER_DIRECTORY }/DATABASE/SURF_MATR   && mkdir -p ${dirSURF}

${OSOAA_ROOT}/exe/OSOAA_MAIN.exe \
        -OSOAA.ResRoot ${dirRESULTS} -OSOAA.Log Trace_Main.Log \
        -OSOAA.Wa 0.440 \
        -ANG.Thetas 30. \
       -AP.Pressure 1023.0  -AP.HR 8.0 -AP.HA 2.0 \
       -AER.Waref 0.550 -AER.AOTref 0.1  \
       -AER.DirMie ${dirMIE_AER} \
       -AER.Model 2 -AER.SF.Model 3 -AER.SF.RH 98.\
       -AER.Log Trace_Aerosols.Log \
       -PHYTO.Chl 0.2 -SED.Csed  0.0 -PHYTO.ProfilType 1 \
       -YS.Abs440 0.00  -DET.Abs440 0.00 \
       -SEA.Depth 15.000 \
       -PROFILE.Log Trace_Profils.Log \
       -PHYTO.ResFile Phyto_Granu.txt -MLP.ResFile MLP_Granu.txt \
       -HYD.DirMie ${dirMIE_HYD}  \
       -HYD.Model 1 \
       -PHYTO.JD.slope 3.0 -PHYTO.JD.rmin 0.01 -PHYTO.JD.rmax 200. \
       -PHYTO.JD.MRwa 1.05 -PHYTO.JD.MIwa -0.000 -PHYTO.JD.rate 1.0 \
       -HYD.Log Trace_hydrosols.Log \
       -SEA.Dir ${dirSURF} -SEA.Ind 1.34  -SEA.Wind 7   \
       -SEA.SurfAlb 0.1  -SEA.BotType 1 -SEA.BotAlb 0.30 \
       -OSOAA.View.Phi 0.0    -OSOAA.View.Level 5\
        -OSOAA.View.Z -10.0   -OSOAA.ResFile.vsVZA RESLUM_vsVZA.txt \
       -OSOAA.View.VZA 0.0  -OSOAA.ResFile.vsZ RESLUM_vsZ.txt \
        -OSOAA.ResFile.Adv.Up   RESLUM_Advanced_UP.txt \
        -SOS.Log Trace_SOS.Log
```

<u>Important warning</u>:

Do not keep any "blank" after the character "\" at end of lines.

3.3.2 How using the GUI (Graphical Unit Interface)

To launch the GUI, in the repertory **$OSOAA_ROOT/ihm/bin** you must execute the script:

runOSOAAI.ksh if using the Korn shell language

runOSOAAI.csh if using the C shell language.

runOSOAAI.bash if using the bash language.

The main window is then loaded.

3.3.2.1 Main window

The first view of the OSOAA GUI shows:

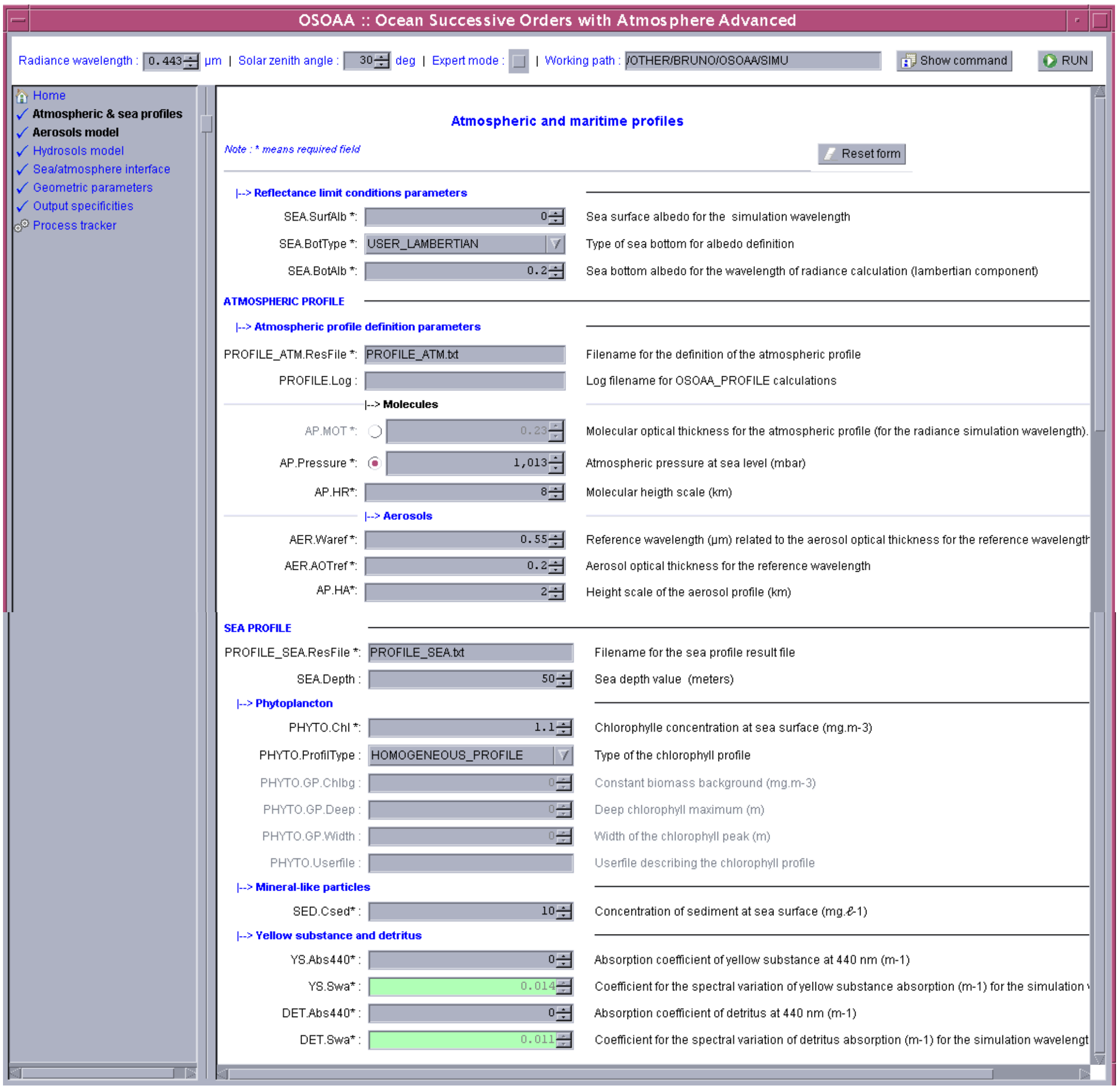
- The top menu bar which defines the general parameters (see section 3.2.1, page 22): the wavelength for radiance calculations, the solar zenith angle and the working path in which will be located the results files.

  The expert mode option is activated by clicking on the related icon. This optional mode allows modifying some default parameters such as the number of angles to perform Gauss quadrature calculation, or such as the maximal order of scattering.

- The left menu bar which allows accessing to the various screens which are devoted to the set of the parameters and to run a simulation.

  For each of these windows, the parameters flagged by an asterix are required. The other ones are optional parameters.

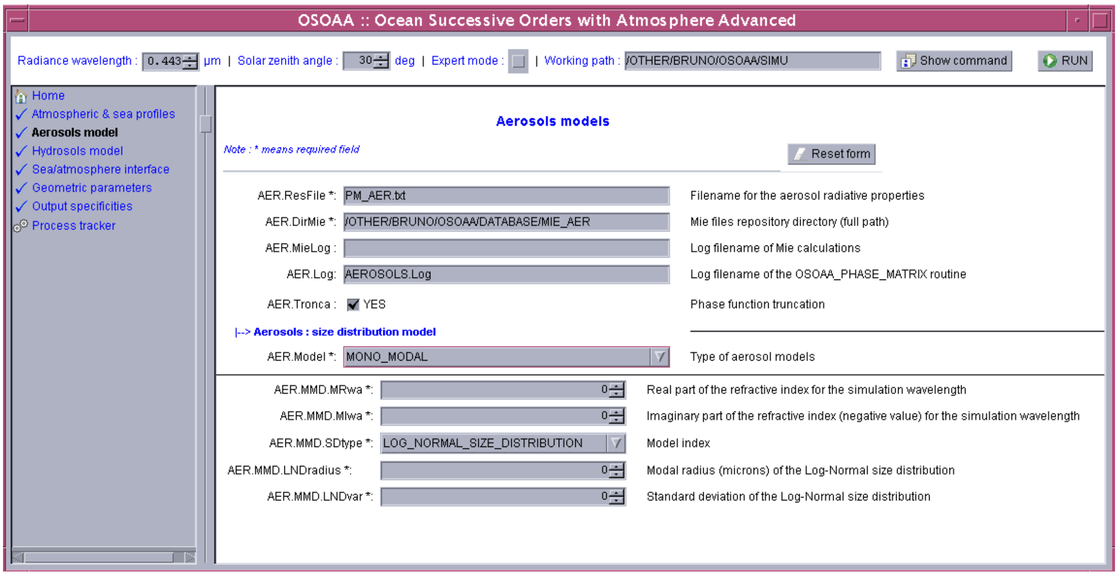
3.3.2.2 Atmospheric and sea profiles



The "Atmospheric and sea profiles" window is devoted to set the parameters related to the surface albedo, to the vertical profile definition of atmospheric constituents (molecules and aerosols optical thicknesses), and to the vertical profile definition of marine constituents (chlorophyll and mineral-like particle concentrations, yellow substance and detritus absorption coefficients).

See the section §3.2.2, from page 23, to get more details on these parameters.

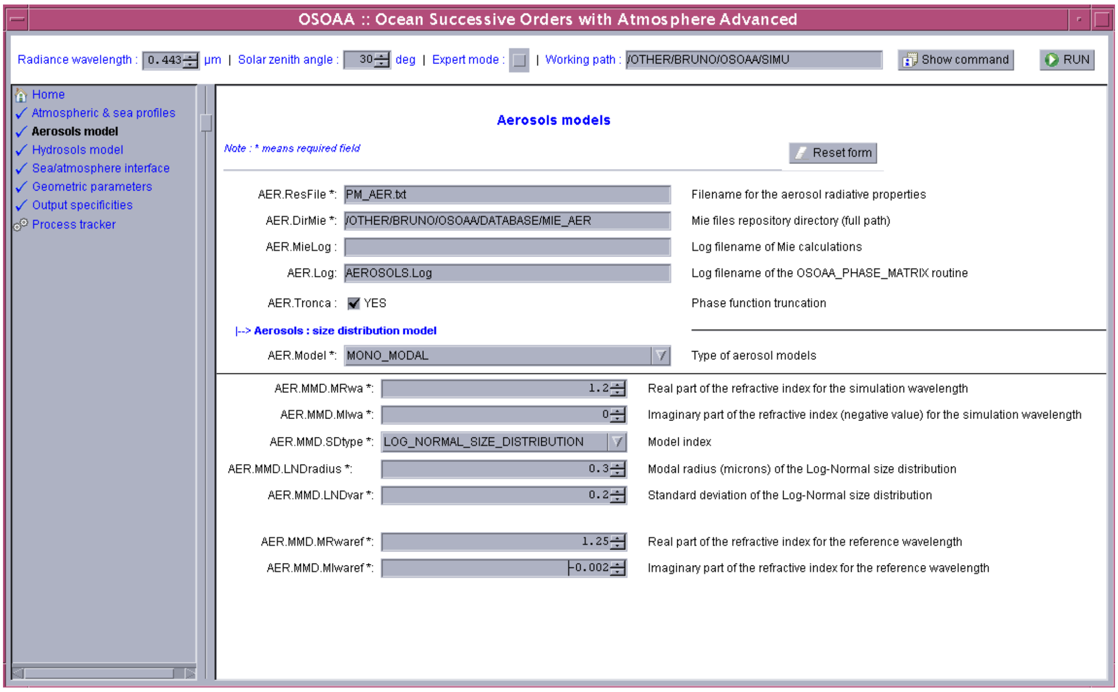
3.3.2.3 Aerosols model



The "Aerosols model" window is devoted to set the parameters related to the type (i.e., composition, size) of the aerosols. See the section §3.2.3, page 27, to get more details on these parameters.

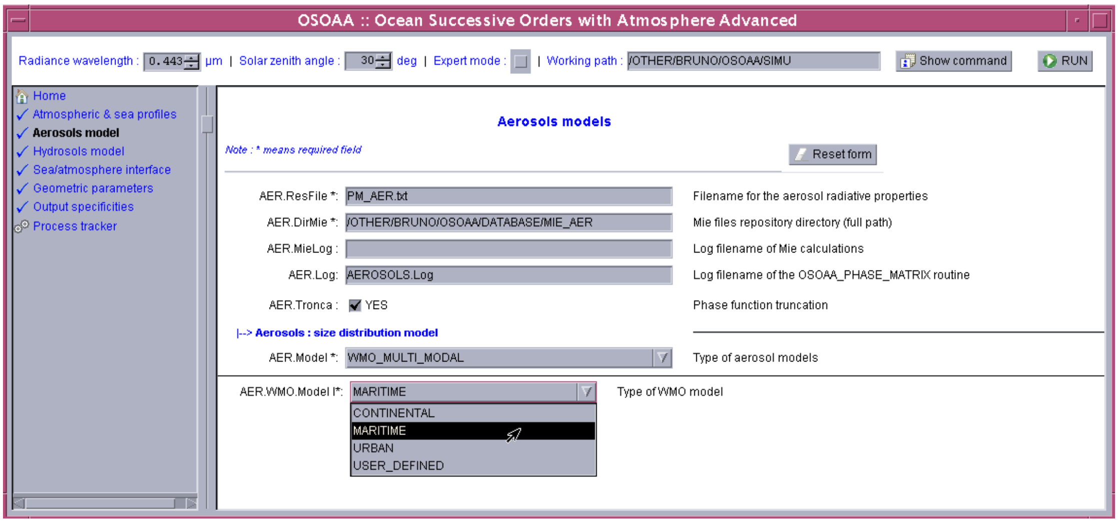
Note: The reference wavelength for aerosols is defined in the "atmospheric and sea profile" window.

Example of Log-Normal aerosol model selection:

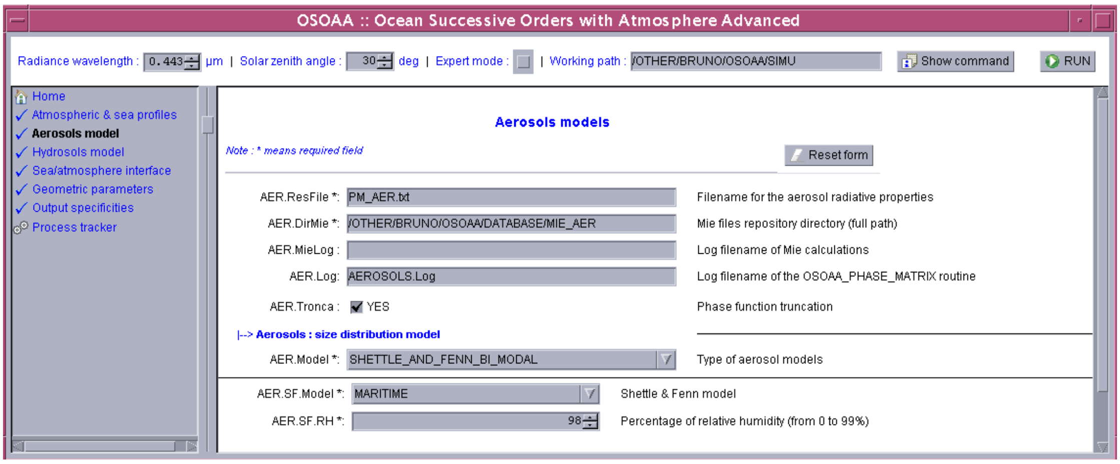


For a mono-modal size distribution model, the user must define the refractive index of particles (real and imaginary parts), both for the wavelength of radiance simulation and for the aerosol reference wavelength (for which is given the AOT defined in the "atmospheric and sea profiles" window).

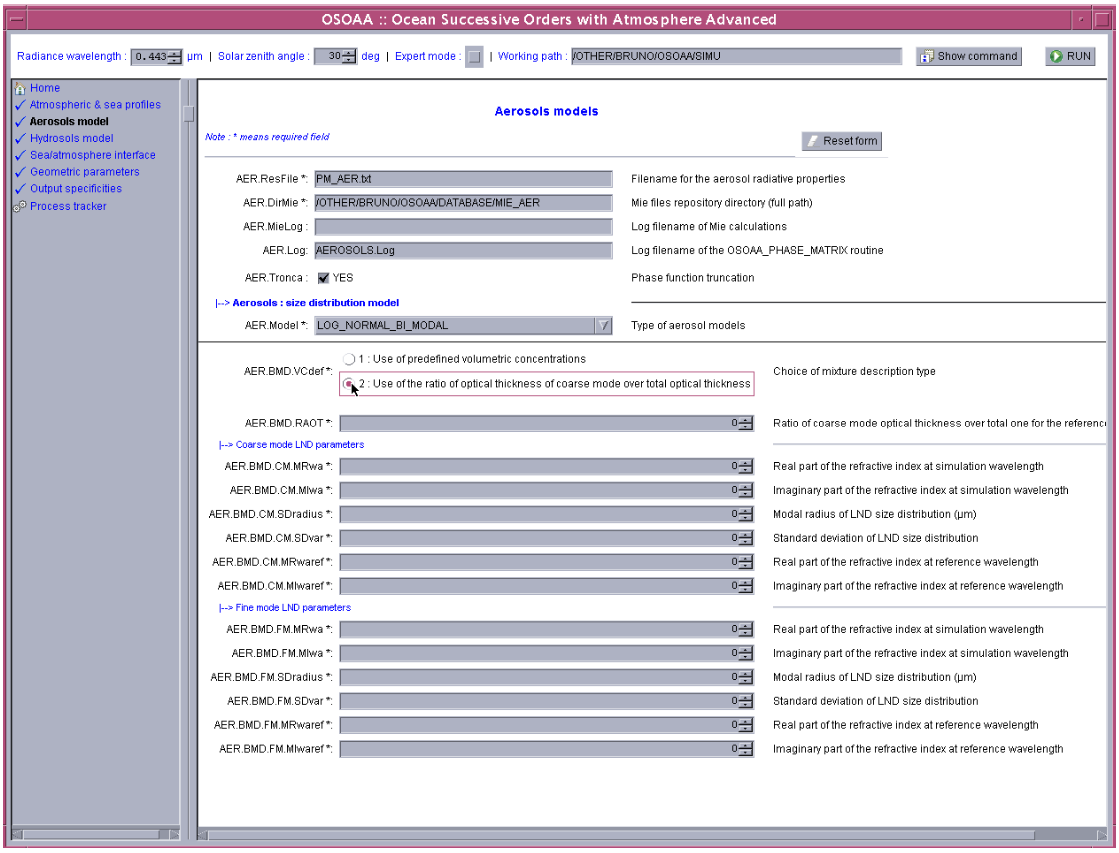
Example of WMO maritime aerosol model selection:



Example of Shettle & Fenn Maritime model selection, for a relative humidity of 98%:

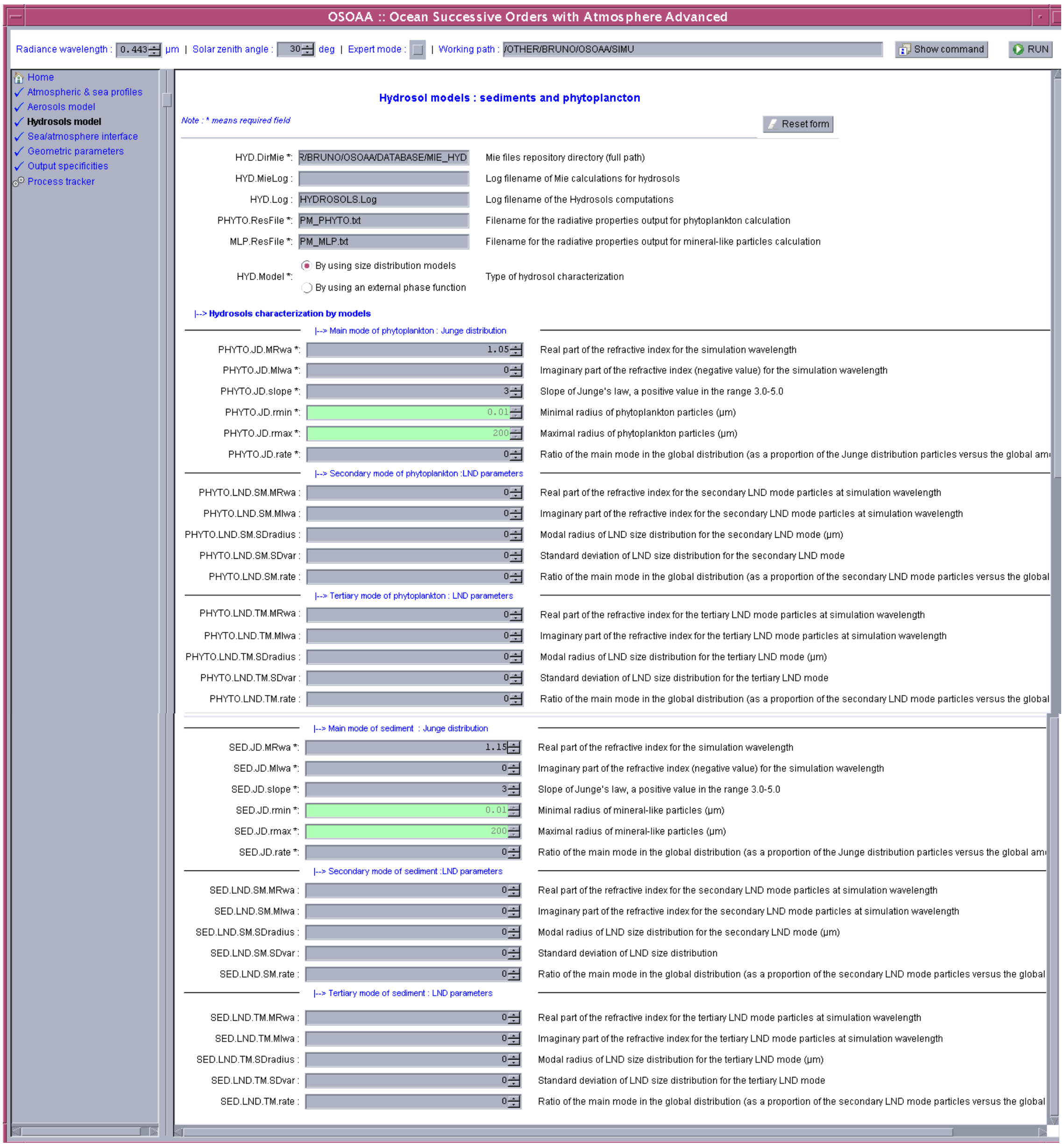


Example of bi-modal Log-Normal aerosol model selection:



The user must define the coarse and fine modes of particles. The refractive index of aerosols must be given both for the wavelength of radiance simulation and for the aerosol reference wavelength (for which is given the AOT defined in the "atmospheric and sea profiles" window).

3.3.2.4 Hydrosols model



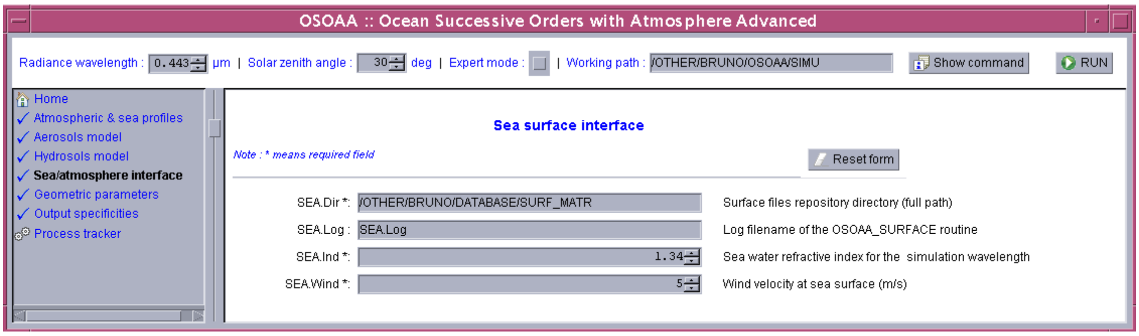
The "Hydrosols model" window is devoted to set the parameters related to the type (i.e., concentration, size distribution) of simulated phytoplankton and mineral-like particles.

Their size distribution can be modelled by three modes: a main Junge's distribution mode, eventually completed by a secondary and a tertiary Log-Normal Distributions.

The refractive index of particles must be given for the wavelength of the radiance simulation.

See the section §3.2.4, page 31, to get more details on these parameters.

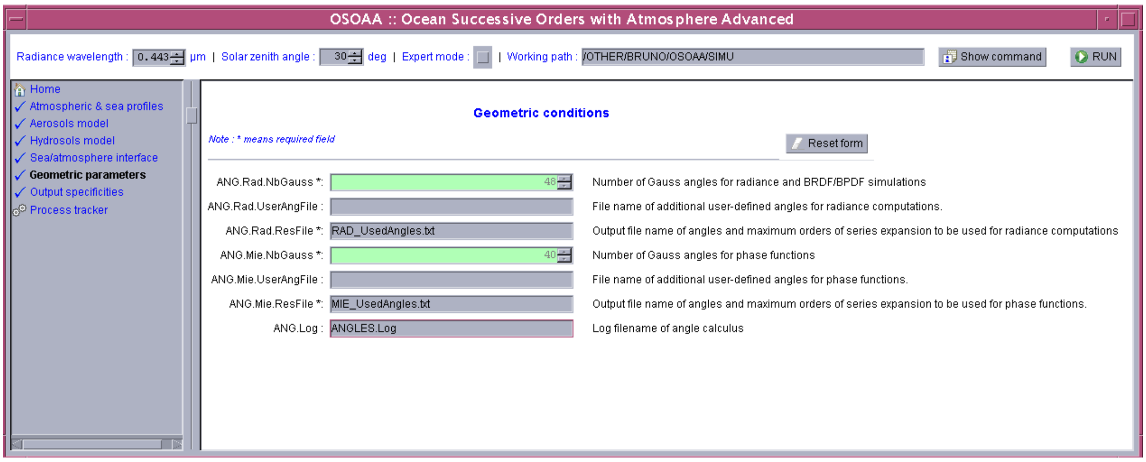
3.3.2.5 Sea/atmosphere interface



The “Sea/atmosphere interface” window is devoted to set the parameters related to the sea interface computation: sea/air refractive index and sea roughness due to the wind velocity at the surface.

See the section §3.2.5, page 37, to get more details on these parameters.

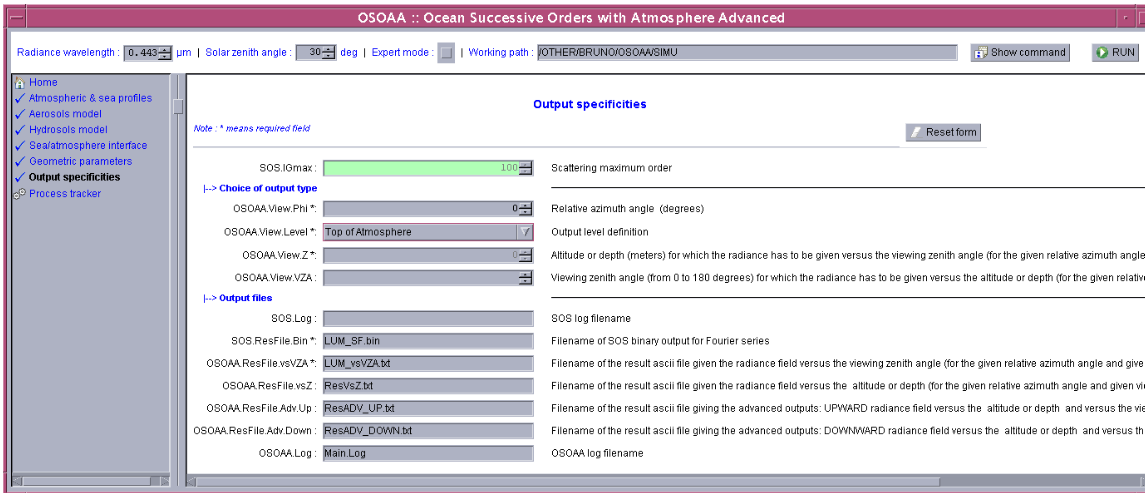
3.3.2.6 Geometric parameters



The “Geometric parameters” window is devoted to define the number of Gauss angles used to i) discriminate the radiance field of view and ii) to compute the particles phase functions. Thanks to this window, the user can also define the location of an own file containing a list of zenith angles for which a radiance simulation is required.

See the section §3.2.6, page 37, to get more details on these parameters.

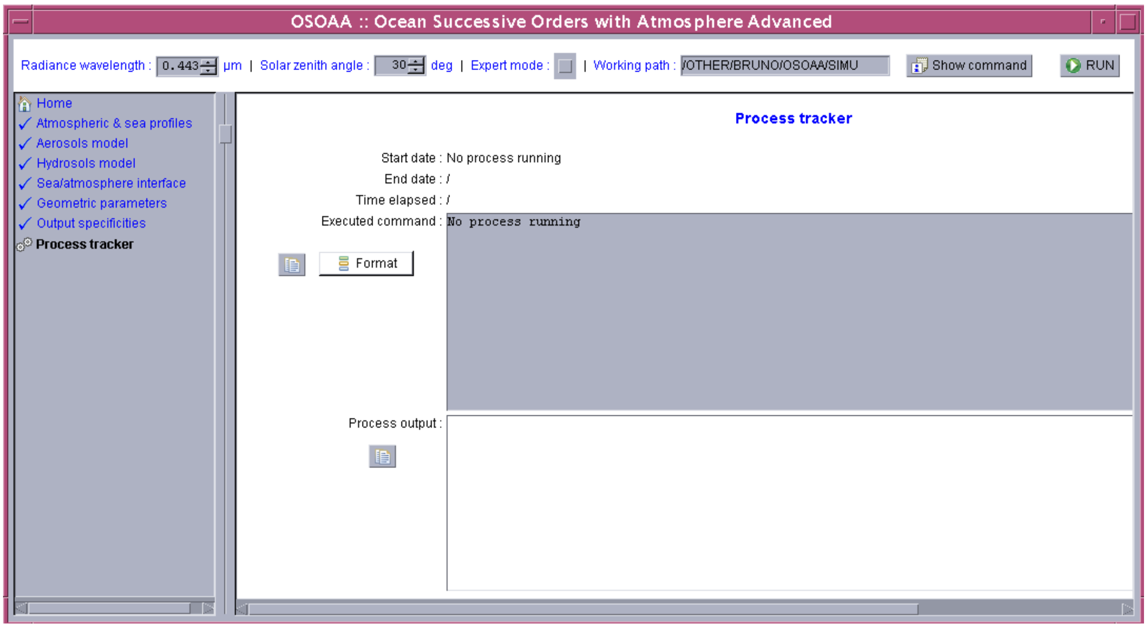
3.3.2.7 Output specificities



The “Output specificities” window defines the type of required outputs: relative azimuth angle, level in the profile for an upwelling radiance field simulation, or zenith angle direction for a radiance profile computation.

See the section §3.2.7, page 39, to get more details on these parameters.

3.3.2.8 Process tracker

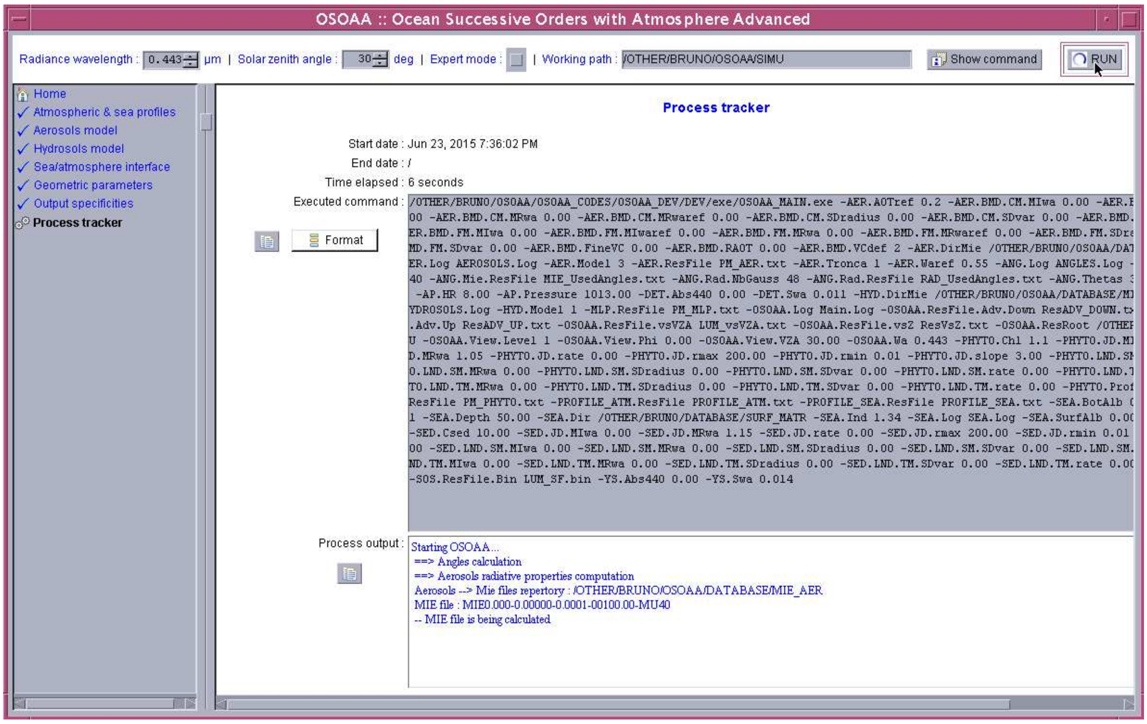


The “Process tracker” window allows executing the defined simulation case, by clicking on the top right icon.

The GUI generates a command file which is run. The command can be shown by selecting the corresponding icon on the top menu bar.

The “Process tracker” screen provides information on the running process.

Example of process information:



3.4 Output files

This chapter describes the content of output files.

The outputs mainly consist of the radiance and degree of polarization simulations. Other files are generated such as files providing the optical thickness profiles or the radiative properties of particles.

3.4.1 Radiance and degree of polarization simulation outputs

The simulation of both radiance and degree of polarization provides two kinds of output files:

- ✓ **Standard output files**:
  - o Filename defined by **-OSOAA.ResFile.vsVZA**:

    This file provides the upwelling radiance field (i.e., the Stokes paramaters I,Q,U where I is the radiance) versus the viewing zenith angle, for the given relative azimuth angle (**-OSOAA.View.Phi**) and for the given altitude or depth (-**OSOAA.View.Z** associated to **-OSOAA.View.Level** equals 5).

    If not defined the default filename in OSOAA.h is applied: CTE_DEFAULT_FICSOS_RES_VS_VZA.

    This ascii file is composed of a header which describes in detail the structure of the file and columns data.
  - o Filename defined by **-OSOAA.ResFile.vsZ**:

    This optional file provides the radiance field (I,Q,U) versus the altitude or depth, for the given relative azimuth angle (**-OSOAA.View.Phi**) and for the given viewing zenith angle (**-OSOAA.View.VZA**).
- ✓ **Advanced output files** provide more detailed information:
  - o The file defined by **-OSOAA.ResFile.Bin** is a binary file containing the (I,Q,U) Stoke's parameters in term of Fourier series expansion. This file is NOT devoted to be used by the user; it is an intermediary file for the computations.

    If not defined the default filename in OSOAA.h is applied: CTE_DEFAULT_FICSOS_RES_BIN.
  - o Filename defined by **-OSOAA.ResFile.Adv.Up** (resp. **Down**):

    This file provides the upwelling (respectively downwelling) Stoke's parameters (I,Q,U) versus the viewing zenith angle and versus the complete profile (depth or altitude), for the given relative azimuth angle (**-OSOAA.View.Phi**).

    For each level of the profile, the radiance field (I,Q,U) is provided for each viewing zenith angle. The scattering angle, the polarization angle and the degree of polarization (also called polarization rate), as well as the polarized intensity are also provided.

Note: The radiance I at level z (or polarized terms Q and U) is normalized to the extra-terrestrial solar irradiance E_{sun} by: π*** I(z) /** E_{sun}

Convention for output zenith angles:

- Sign convention applied on zenith angles :
  - The viewing angle is positive in the half-plane of relative azimuth ϕ.
  - It is negative in the half-plane $\phi+\pi$.

  Note that the convention used for the value of the azimuth is opposite to the geographical definition of the azimuth.

  For instance, in the solar principal plane:

  Azimuth = 180° means that the Satellite and the Sun are located in the same half-plane. In this case the viewing zenith angle (VZA) is negative.

  Azimuth = 0° means that the Satellite and the Sun are located in opposite half-planes with respect to the zenith direction. In this case the viewing zenith angle (VZA) is positive.

- Angles values:
  - For the upward radiance, the viewing angle is zero when looking up towards the zenith.
  - For the downward radiance, the viewing angle is zero when looking down at nadir.
  - The viewing angle is ± 90° for the horizon.

Figure 1 provides a schematic of the convention used for the sign of the zenith angles.
For a given level of the atmospheric or marine profile, this figure illustrates the viewing angle θ_k corresponding to a direction k and the associated sign, for the following cases:

Aera A on Figure 1: Upward direction for a relative azimuth ϕ equals to the value defined by the user (-**OSOAA.View.Phi**)	$\theta_k > 0$ Propagation toward the zenith: $\theta = 0°$ Propagation toward the horizon: $\theta = 90°$
Aera D: Downward direction for a relative azimuth ϕ equals to the value defined by the user	$\theta_k > 0$ Propagation toward the nadir: $\theta = 0°$ Propagation toward the horizon: $\theta = 90°$

Aera B: Upward direction for a relative azimuth **ϕ + 180°** (value defined by the user plus 180°)	$\theta_k < 0$ Propagation toward the zenith: $\theta = 0°$ Propagation toward the horizon: $\theta = -90°$
Aera C: Downward direction for a relative azimuth **ϕ + 180°** (value defined by the user plus 180°)	$\theta_k < 0$ Propagation toward the nadir: $\theta = 0°$ Propagation toward the horizon: $\theta = -90°$

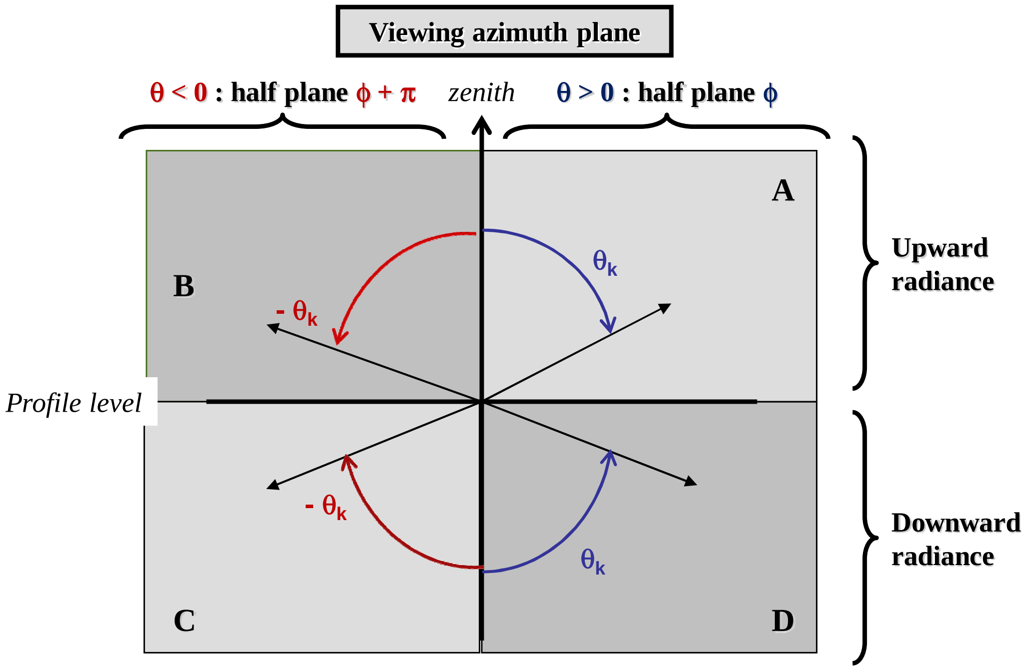


Figure 1 : Convention on zenith angles values for the upwelling and downwelling radiance field. A direction k is illustrated for an upward or downward direction of light propagation. The configuration is shown for each half plane of the relative azimuth, namely ϕ and ϕ+180,°is also presented in the figure.

Figure 2 illustrates the location of the sun in the solar principal plane and the associated solar zenith θ_s angle as defined by the user (**-ANG.Thetas**). Let's notice that the solar incident direction is actually a downward direction. As a result, the solar angle used for inner computations is redefined as being 180° - θ_s.

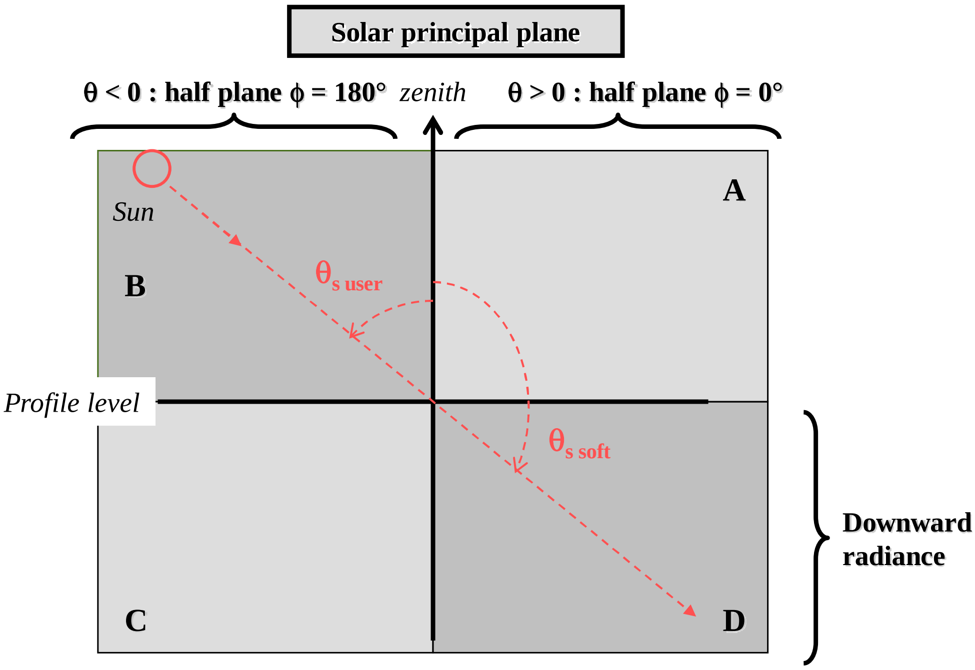


Figure 2 : Location of the Sun in the solar principal plane (ϕ = 180°). Representation of the solar zenith angle defined by the user and of the solar angle as used by the software with respect to the zenith direction and to the incident direction of the solar beam.

Example of standard output: Filename defined by -OSOAA.ResFile.vsVZA

```
STANDARD RESULTS :
   UPWARD RADIANCE FIELD VERSUS THE VIEWING ZENITH ANGLE
   (RELATIVE AZIMUTH AND ALTITUDE/DEPTH ARE FIXED)
 ----------------------------------------------------------------------------------------------
 Relative azimuth (degrees) :

    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

    Simulated relative azimuth (degrees) :
        for VZA < 0 (sign convention):  180.
        for VZA > 0 (sign convention):  0.

 Sea depth (m) : -10.

 Columns parameters :
   VZA      :  Viewing Zenith Angle (deg)
   SCA_ANG :  Scattering angle (deg)
   I        :  Stokes parameter at output level Z
               normalized to the extraterrestrial solar irradiance (PI * L(z) / Esun)
   REFL     :  Reflectance at output level Z (PI * L(z) / Ed(z))
   POL_RATE:  Degree of polarization (%)
   LPOL     :  Polarized intensity at output level Z
               normalized to the extraterrestrial solar irradiance (PI * Lpol(z) / Esun)
   REFL_POL:  Polarized reflectance at output level Z (PI * Lpol(z) / Ed(z))
 ----------------------------------------------------------------------------------------------
   VZA    SCA_ANG       I            REFL         POL_RATE      LPOL         REFL_POL
 -89.07   112.84   0.911432E-12  0.128177E-02    64.18   0.584976E-12  0.822669E-03
 -87.20   114.71   0.873536E-12  0.122848E-02    63.11   0.551277E-12  0.775277E-03
 -85.34   116.57   0.835169E-12  0.117452E-02    62.13   0.518909E-12  0.729757E-03
   •
   •
```

Example of standard output: Filename defined by -OSOAA.ResFile.vsZ

```
STANDARD RESULTS :
   RADIANCE FIELD VERSUS THE SEA DEPTH
   (RELATIVE AZIMUTH AND VIEWING ZENITH ANGLE ARE FIXED)
 ----------------------------------------------------------------------------------------------
 Relative azimuth (degrees) :

    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

    Simulated relative azimuth (degrees) :  0.

 Upward direction VZA (degrees) :  0.

 Columns parameters :
   Z        :  Sea depth (meters)
   SCA_ANG :  Scattering angle (deg)
   I        :  Stokes parameter at level Z
               normalized to the extraterrestrial solar irradiance (PI * L(z) / Esun)
   REFL     :  Reflectance at level Z (PI * L(z) / Ed(z))
   POL_RATE:  Degree of polarization (%)
   LPOL     :  Polarized intensity at level Z
               normalized to the extraterrestrial solar irradiance (PI * Lpol(z) / Esun)
   REFL_POL:  Polarized reflectance at level Z (PI * Lpol(z) / Ed(z))
 ----------------------------------------------------------------------------------------------
       Z      SCA_ANG        I             REFL        POL_RATE      LPOL          REFL_POL
   0.00000   158.09   0.518880E-03  0.689353E-03     8.16   0.423537E-04  0.562686E-04
   0.00000   158.09   0.518829E-03  0.689355E-03     8.16   0.423496E-04  0.562688E-04
  -0.18300   158.09   0.353436E-03  0.689475E-03     8.15   0.287944E-04  0.561715E-04
  -0.36700   158.09   0.240677E-03  0.689471E-03     8.12   0.195526E-04  0.560129E-04
   •
   •
```

Example of advanced output: Filename defined by -OSOAA.ResFile.Adv.Up

```
ADVANCED RESULTS : UPWARD RADIANCE FIELD
            VERSUS ALTITUDE / DEPTH
            AND VERSUS THE VIEWING ZENITH ANGLE
            (RELATIVE AZIMUTH IS FIXED)
 --------------------------------------------------------------------------------------------------------
 Relative azimuth (degrees) :

    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

    Simulated relative azimuth (degrees) :
        for VZA < 0 (sign convention):  180.
        for VZA > 0 (sign convention):  0.

 Columns parameters :
   LEVEL    :  Level I of the profile
                 TOA is level 0
                 0+ (over surface) is level  26
                 0- (under surface) is level 27
   Z        :  Altitude or depth (meters)
   VZA      :  Viewing Zenith Angle (deg)
   SCA_ANG  :  Scattering angle (deg)
   I, Q, U  :  Stokes parameters at level Z
               normalized to the extraterrestrial solar irradiance (PI * L(z) / Esun)
   POL_ANG  :  Polarization angle (deg)
   POL_RATE:   Degree of polarization (%)
   LPOL     :  Polarized intensity at level Z
               normalized to the extraterrestrial solar irradiance (PI * Lpol(z) / Esun)
 --------------------------------------------------------------------------------------------------------
  LEVEL     Z          VZA     SCA_ANG        I              Q              U          POL_ANG POL_RATE     LPOL
   0    300000.000   -89.07   120.93   0.349414E+00  -0.153293E+00   0.224678E-16    90.00    43.87    0.153293E+00
   0    300000.000   -87.20   122.80   0.356478E+00  -0.143248E+00   0.216680E-16    90.00    40.18    0.143248E+00
   •
```

3.4.2 Files defining the angles used for calculations

3.4.2.1 Angles used for radiance calculations

OSOAA generates files containing the information about the angles used to compute both phase functions and radiance fields. They are located in the subdirectory ***Advanced_Output***.

The file defined by **-ANG.Rad.Resfile** is used for the radiance computations. It contains the list of Gauss angles used for spatial integration calculations, and associated weights, as well as the list of angles added by the user (from the file defined by **-ANG.Rad.UserAngFile)**.

This file also provided information on the solar zenith angle both in the air and in the sea and the corresponding angle indices IMUS and IMUSW). It defines the maximal orders of series expansions, for inner computations (OS_NB, OS_NS and OS_NM).

NB_TOTAL_ANGLES	Total number of angles to be used
NB_GAUSS_ANGLES	Number of Gauss angles
ANGLES_USERFILE	Filename for user-defined angles (NO_USER_ANGLES if no file).
SOLAR ZENITH ANGLE	Solar zenith angle (degrees) in the air
INTERNAL_IMUS	Index number in the angles array for solar zenith angle
TRANSMITTED SOLAR ZENITH ANGLE IN WATER	Solar zenith angle (degrees) in the sea
INTERNAL_IMUSW	Index number in the angles array for solar zenith angle
INTERNAL_OS_NB	Maximum order for expansion of phase functions as Legendre polynomials
INTERNAL_OS_NS	Maximum order of the Legendre polynomials for the Fresnel matrix elements and Fourier series for the radiance.
INTERNAL_OS_NM	Maximum order of the Fourier series for the wave probability G function which acts as a weight factor on the Fresnel matrix during computation of the reflection matrices.
INDEX COS_ANGLE WEIGHT OUTPUT • • •	For each line: angle index, cosine, weight, and whether the angle is a user's defined: (1) if yes, (0) if no. Format: I4, 1X, 2D21.14, 1X, I4.

Example of a file defining the angles used to compute radiance:
Filename defined by -ANG.Rad.Resfile

The OUTPUT column gives the information about the angle status : OUTPUT = 1 means there is a radiance calculation provided in the output files for this angle; if OUTPUT = 0, there is no radiance calculation for this angle..

```
NB_TOTAL_ANGLES :   51
NB_GAUSS_ANGLES :   48
ANGLES_USERFILE :NO_USER_ANGLES
SOLAR ZENITH ANGLE : 30.000
INTERNAL_IMUS :   19
TRANSMITTED SOLAR ZENITH ANGLE IN WATER : 21.909
INTERNAL_IMUSW :   13
INTERNAL_OS_NB :   80
INTERNAL_OS_NS :   96
INTERNAL_OS_NM : 176
INDEX    COS_ANGLE             WEIGHT              OUTPUT
   1  0.10000000000000E+01 0.00000000000000E+00    1
   2  0.99968950388323E+00 0.79679206555877E-03    1
   3  0.99836437586318E+00 0.18539607889415E-02    1
   4  0.99598184298721E+00 0.29107318179379E-02    1
   5  0.99254390032376E+00 0.39645543384447E-02    1
   6  0.98805412632962E+00 0.50142027429294E-02    1
   7  0.98251726356301E+00 0.60585455042351E-02    1
   8  0.97593917458514E+00 0.70964707911542E-02    1
   9  0.96832682846326E+00 0.81268769256985E-02    1
  10  0.95968829144874E+00 0.91486712307830E-02    1
   •
   •
   •
```

3.4.2.2 Angles used for Mie phase function calculations

The file defined by **-ANG.Mie.Resfile** is used for the Mie computations. Its content is similar as that of a radiance computation. The list of angles includes the Gauss angles (and associated weights), as well as the list of potential angles added by the user (from the file defined by **-ANG.Mie.UserAngFile)**.

NB_TOTAL_ANGLES	Total number of angles to be used
NB_GAUSS_ANGLES	Number of Gauss angles
ANGLES_USERFILE	Filename for user-defined angles (NO_USER_ANGLES if no file).
INTERNAL_OS_NB	Maximum order for expansion of phase functions as Legendre polynomials
INDEX COS_ANGLE WEIGHT • • •	For each line: angle index, cosine and weight. Format: I4, 1X, 2D21.14, 1X, I4.

Example of a file defining the angles used to compute phase functions:
Filename defined by -ANG.Mie.Resfile

```
NB_TOTAL_ANGLES :   41
NB_GAUSS_ANGLES :   40
ANGLES_USERFILE :NO_USER_ANGLES
INTERNAL_OS_NB :   80
INDEX    COS_ANGLE            WEIGHT
    1  0.19511383256794E-01 0.39017813656307E-01
    2  0.58504437152421E-01 0.38958395962770E-01
    3  0.97408398441585E-01 0.38839651059052E-01
    4  0.13616402280914E+00 0.38661759774076E-01
    5  0.17471229183265E+00 0.38424993006959E-01
    6  0.21299450285767E+00 0.38129711314478E-01
    7  0.25095235839227E+00 0.37776364362001E-01
    8  0.28852805488451E+00 0.37365490238731E-01
    9  0.32566437074770E+00 0.36897714638276E-01
   10  0.36230475349949E+00 0.36373749905836E-01
   11  0.39839340588197E+00 0.35794393953416E-01
    •
    •
```

3.4.3 Files defining the sea and atmosphere optical thickness profiles

OSOAA generates the optical thickness vertical profile both for the atmosphere and for the sea layers.

Sea optical thickness profile file : PROFILE_SEA	
Param.	User definition : **-PROFILE_SEA.ResFile** Default filename: **CTE_DEFAULT_FICPROFIL_SEA_RES**
Location	Directory ***Advanced_Output/*** in the working folder **(–OSOAA.ResRoot)**
Content	This file contains the sea optical thickness vertical profile calculated by OSOAA. For each line, this file provides: • the **level number (or index)** p • the **depth of level** p (in meters) • the **extinction optical thickness** for the **level p**, • the **scattering mixing rate** of pure sea water for the **layer p** • the **scattering mixing rate** of phytoplankton for the **layer p** • the **scattering mixing rate** of Mineral-Like particles for the **layer p** Note that the radiative parameters define the real profile **without any adjustment to the phase function truncation** of the components.
Format	Ascii file. **I5, 1X, F9.3, 1X, E14.7, 1X, 3(1X, F7.5)**

Atmospheric optical thickness profile file : PROFILE_ATM	
Param.	User definition : **-PROFILE_ATM.ResFile** Default filename: **CTE_DEFAULT_FICPROFIL_ATM_RES**
Location	Directory ***Advanced_Output/*** in the working folder **(–OSOAA.ResRoot)**
Content	This file contains the atmospheric optical thickness vertical profile calculated by OSOAA. For each line, this file provides: • the **level number (or index)** k • the **altitude of level** k (in km) • the **extinction optical thickness** for the **level k**, • the **scattering mixing rate** of aerosols for the **layer k** • the **scattering mixing rate** of air molecules for the **layer k** The radiative parameters define the real profile **without any adjustment to the aerosol phase function truncation**.
Format	Ascii file. **2X, I4, F9.3, 3(1X, F9.5)**

3.4.4 Files defining the radiative properties of particles

OSOAA generates files containing the radiative properties of particles: aerosols, phytoplankton and mineral-like particles. These files are used by OSOAA to compute the radiance.

Files containing the radiative properties of Aerosols, chlorophyll or Mineral-Like particles	
Param.	User definition : **-AER.ResFile**, **-PHYTO.ResFile** or **-MLP.ResFile** Default filename: **CTE_DEFAULT_FICGRANU_AER** **CTE_DEFAULT_FICGRANU_PHYTO** **CTE_DEFAULT_FICGRANU_MLP**
Location	Directory ***Advanced_Output/*** in the working folder **(–OSOAA.ResRoot)**
Content	First thirteen header lines provide comments and formatted data on the extinction and scattering cross-sections (in μm^2), the asymmetry factor, the volume of the equivalent mean particle (in μm^3), the real part of the mean refractive index, the phase function truncation coefficient and the single scattering albedo (adjusted to the truncation). The following lines contains the phase matrix coefficients of the development of the Legendre Polynomials of the phase matrix for each order k ranging from k= 0 up to the maximum order of computations (OS_NB). For each line, this file provides: • the **coefficient α(k)** Related to the polarised phase functions • the **coefficient β(k)** Related to the intensity phase function • the **coefficient γ(k)** Related to the polarised phase functions • the **coefficient ξ(k)** Related to the polarised phase functions These coefficients are **adjusted to a phase function truncation** if applied.
Format	Ascii file. **E15.8, 3(1X, E15.8)** for lines of matrix phase function coefficients

3.4.5 Log files

The different logfiles are listed in Table 10.

All of them are optionally produced under the request of the user.

As the production of logfiles from Mie computations and interface matrices calculations are time consuming, it is suggested to produce them only if strictly necessary.

Table 10 : List of logfiles

Logfile parameter	Contents
-OSOAA.Log	The main logfile gives information on the different routines execution (input/output parameters, warnings, error cases, …)
-ANG.Log	This logfile gives information about the angles computations: Gauss angles used for the phase functions and radiance calculations, solar zenith angle in the air and sea, user's angles.
-PROFILE.Log	This logfile gives information about the atmospheric and marine profiles computation.
-AER.Log	This logfile gives information about the radiative properties computation for aerosols: phase function of each elementary components, mixed-average phase function, truncation calculations, scattering and extinction cross-sections.
-AER.MieLog	This logfile gives the value of matrix phase function (polarized form) versus the size parameter from Mie calculations.
-HYD.Log	As for aerosols, this logfile gives information about the radiative properties computation for hydrosols.
-HYD.MieLog	As for aerosols, this logfile gives information about the Mie computations for hydrosols.
-SEA.Log	This logfile gives information about the calculation of interface matrices (RAA, RWW, TAW, TWA): Fresnel matrices, probability function of the waves orientation,…
-SOS.Log	This logfile gives information about the successive orders of scattering computation (core of the radiative transfer code).

3.5 Input user files

3.5.1 User file for angles definition

The file defined by **-ANG.Rad.UserAngFile** contains a list of zenith angles for which the user wants to get a radiance simulation.

Its first line aims at defining if the user requires getting output radiance fields covering all the angles (Gauss angles and user's ones) or only the user's angles provided in the file:

- for all the angles (Gauss angles and user's ones) → `OUTPUT_GAUSS_ANGLES=1`
- or only for the user's angles → `OUTPUT_GAUSS_ANGLES=0`

Example of a user's angles file defined by -ANG.Rad.UserAngFile
In this example, only the radiance calculated for the user's angles will be provided in radiance output files (presented in section 3.4.1).

```
OUTPUT_GAUSS_ANGLES=0
20
25
30
35
40
```

The file defined by **-ANG.Mie.UserAngFile** contains a list of scattering angles for which the user wants to get a value of phase function simulations. Only the logfiles for aerosol and hydrosol computations are concerned by this addition of angles to the Gauss angles.

> Note: The list of angles must include values θ_{user} up to 90°.
> OSOAA adds the complementary angles 180°-θ_{user}.

Example of a user's angles file defined by -ANG.Mie.UserAngFile

```
10
20
30
40
50
60
```

> Important note:
>
> **The filename for a list of user's angles must be changed if the list of angle changes.**
>
> Indeed, Mie files and interface files (BRDF, BPDF matrices) are stored in files for which their names include the filename of user's angles. They are not recalculated if a Mie file or and interface file with the same name has already been created.

3.5.2 User file for the chlorophyll profile

The user can use its own chlorophyll profile defined in the file **PHYTO.Userfile**.

This file must provide the chlorophyll concentration for a set of sea depths.

Format for each line: Z_user Chl_user

(sea depth in meters, chlorophyll concentration in mg.m^{-3}).

The maximal number of lines cannot exceed the value of the parameter CTE_NBWA_MAX (defined in the OSOAA.h file).

The first value Z_user must be 0 (surface) and the last value must exceed the sea depth (provided by the user or the euphotic depth calculated by OSOAA)

3.5.3 User file for the aerosol or hydrosol radiative properties

The user can use aerosol radiative properties (phase function, extinction and scattering cross-sections) from an external source, as well as for hydrosols.

The corresponding files are defined by **-AER.ExtData** and **-HYD.ExtData**.

The format of these files is based on the Oleg Dubovik's tool called DLS [DR6] which provides the primary scattering properties of homogeneous spheroid particles with random orientation. However, the first lines of this format have been revised for OSOAA purposes.

These Ascii files must contain:

1st line: **EXTINCTION_COEF : *Value***
format : real value unformatted

Values : extinction cross-section (µm^{-2})

Note : the value is interpreted as the second part of the line after the ":"

2nd line: **SCATTERING_COEF : *Value***
format : real value unformatted

Value : scattering cross-section (µm^{-2}).

Note : the value is interpreted as the second part of the line after the ":"

3rd line: **NB_LINES : *Value***
format : integer value unformatted

Value : Number of angles describing the user's phase functions.

Note : the value is interpreted as the second part of the line after the ":"

It can not exceed the value CTE_MAXNB_ANG_EXT (in OSOAA.h).

4th line: Comments

Lines 5 to (5+NB_LINES-1) : **ANGLE F11 -F12/F11 F22/F1 F33/F11**
format : real values unformatted

Value: ANGLE : scattering angle in degrees
F11 : phase function in intensity P_{11}
-F12/F11 : ratio of functions $-P_{12}$ and P_{11}
F22/F11 : ratio of functions P_{22} and P_{11}
F33/F11 : ratio of functions P_{33} and P_{11}

> Sign convention: the F_{12} function is negative for Rayleigh scattering. It is the same convention as in the internal OSOAA code.

The next lines are not read.

Example of a user's phase function data defined by -AER.ExtData

```
EXTINCTION_COEF : 5.43712E-02
SCATTERING_COEF : 5.39636E-02
NB_LINES : 99
Angle        F11          -F12/F11     F22/F11      F33/F11
180.00       4.190E-01     0.000E+00   1.000E+00    -1.000E+00
178.57       3.522E-01     6.297E-02   1.000E+00    -6.856E-01
176.72       3.175E-01    -5.297E-02   1.000E+00    -2.274E-01
174.86       2.848E-01    -1.160E-01   1.000E+00    -2.901E-02
    •
    •
    •
```

4. Theory and Methodology

This chapter outlines the details of the theory and equation that are used to solve the radiative transfer equation using the successive orders of scattering method within the OSOAA model.

4.1 Radiance computations

4.1.1 Successive orders calculations

Figure 3 shows the different terms of light interaction which are modelled by OSOAA. Starting from the direct solar beam illumination, each order of scattering is successively considered by calculating all the light interactions affecting the radiance field: scattering and absorption in the sea and air environments, reflection and transmission on the sea surface.

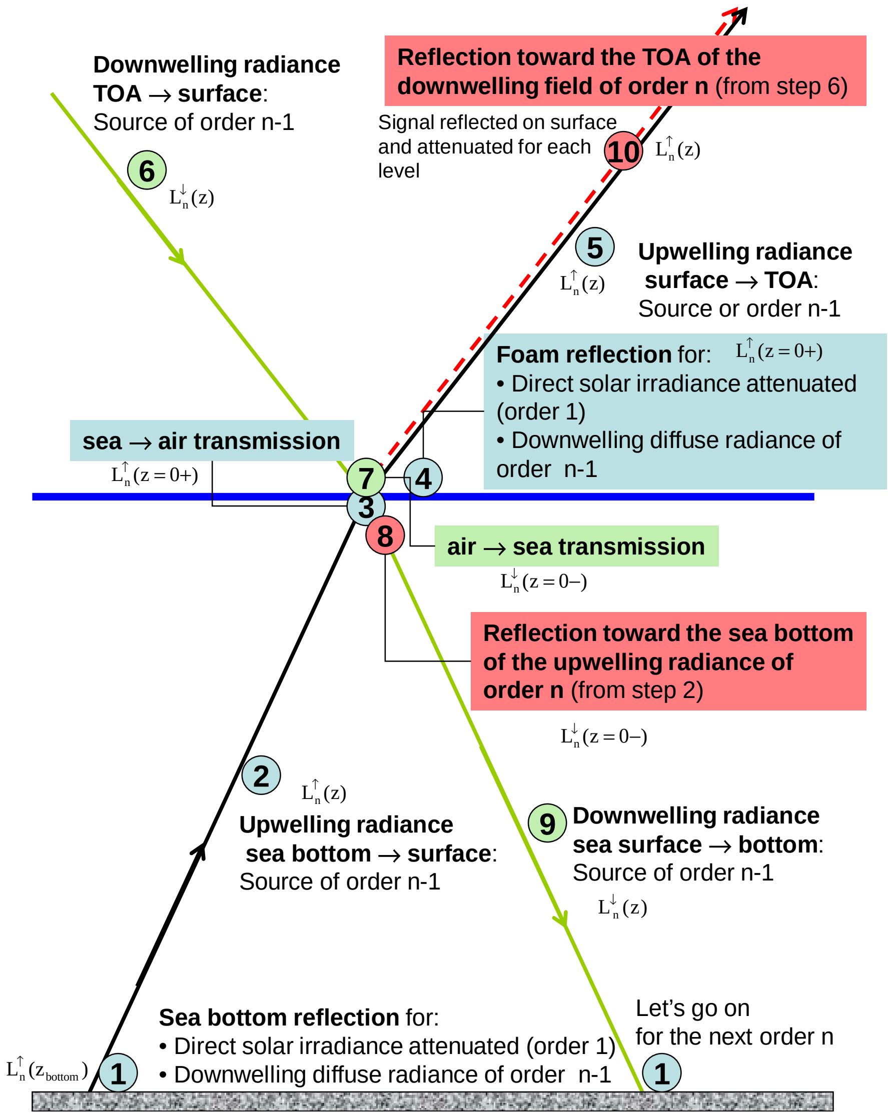


Figure 3 : Light interactions for the order n of successive orders

<u>Source functions calculation:</u>

Atmospheric source function:

- Scattering cores: molecules and aerosols.
- For the order 1: scattering of the direct solar beam, attenuated by the atmosphere. Calculations also include the scattering of the direct solar beam following its reflection on the surface, in case of a flat sea (if wind velocity is null).
- For the order n>1: scattering of radiance field of order n-1.

Marine source function:

- Scattering cores: water molecules, chlorophyll and mineral-like particles.
- For the order 1: scattering of the direct solar beam, refracted in the sea and attenuated through the atmosphere and sea.
- For the order n>1: scattering of the radiance field of order n-1.

<u>Calculation of the upwelling radiance field:</u>

1) Calculation of the **radiance reflected at the sea bottom**
   - Order 1: lambertian reflection of the direct solar beam reaching the sea bottom (refracted in the sea and attenuated through the atmosphere and sea).
   - Order n: lambertian reflection of the downwelling radiance of n-1.
2) Calculation of the **upwelling radiance field from the bottom to the sea surface** (level 0-, just below the surface): vertical integration of each layer contributions, throughout the marine profile.
3) Calculation of the **upwelling radiance transmitted by the sea → air interface** (from level 0- to level 0+, just above the sea surface)
4) Addition of the **foam lambertian reflection**
   - Order 1: <u>lambertian</u> reflection on the foam of the direct solar beam reaching the sea surface.
   - Order n: <u>lambertian</u> reflection on the foam of the radiance field of order n-1.
5) Calculation of the **upwelling radiance field from the sea surface to TOA**: vertical integration of each layer contributions, throughout the atmospheric profile.

<u>Calculation of the downwelling radiance field:</u>

6) Calculation of the **downwelling radiance field from TOA to the sea surface**: vertical integration of each layer contributions, throughout the atmospheric profile.
7) Calculation of **downwelling radiance transmitted by the sea surface interface** (from air to sea).

8) Addition of the **reflection toward the sea bottom of the upwelling marine light** (from step 2 of the current order n)

9) Calculation of the **downwelling radiance field from the sea surface to the sea bottom:** vertical integration of each layer contributions, throughout the marine profile.

Complementary contribution to the upwelling radiance field:

10) Addition of the upward reflection on sea surface of the atmospheric downwelling radiance field (calculated by step 6 of current order n).

4.1.2 Fourier series expansion of Stokes parameters

The Stokes parameters are commonly used to characterize the state of polarization.

For an optical thickness τ in the atmospheric or marine profile, and for a light propagation toward the direction (μ,ϕ), we define the Stokes vector by:

$$\overline{L}(\tau,\mu,\phi)=\begin{pmatrix} I(\tau,\mu,\phi) \\ Q(\tau,\mu,\phi) \\ U(\tau,\mu,\phi) \end{pmatrix} \qquad (1)$$

for the zenith angle θ (μ = cos θ) and the azimuth angle ϕ.

> Notes:
>
> - OSOAA calculates radiance I (or polarized terms Q and U) normalized to the extra-terrestrial solar irradiance E_{sun} by: $\boldsymbol{\pi * I / E_{sun}}$
> - OSOAA does not calculate the Stokes parameter V, as the ellipticity of the polarized light is generally very small in the atmosphere and ocean; thus, it is often neglected.

The Stoke vector is expanded into Fourier series of the azimuth in order to separate the variables μ and ϕ, and to make faster the calculations, by:

$$\overline{L}(\tau,\mu,\phi)=\begin{pmatrix} I(\tau,\mu,\phi) \\ Q(\tau,\mu,\phi) \\ U(\tau,\mu,\phi) \end{pmatrix}=\sum_{s=0}^{S}(2-\delta_{0s})\times\begin{pmatrix} \cos(s\phi)\times\sum_n I_n^s(\tau,\mu) \\ \cos(s\phi)\times\sum_n Q_n^s(\tau,\mu) \\ \sin(s\phi)\times\sum_n U_n^s(\tau,\mu) \end{pmatrix} \qquad (2)$$

where:

- I, Q and U are the Stokes parameters,
- τ is the optical thickness in the profile in the atmosphere or in the ocean,

- μ is the cosine the zenith angle of the propagation direction (positive or negative value),
- ϕ is the azimuth angle of the propagation direction (relative to the solar azimuth),
- s is the order of the Fourier series expansion, S is the maximal order.
- n is the order of interaction (scattering or air/sea surface interaction with light),
- the function $\delta_{0S} = 1$ if s = 0, otherwise $\delta_{0S} = 0$.

For each order **s** of the Fourier series expansion, OSOAA accumulates the successive orders **n** of interaction:

$$\overline{L}^{s}(\tau,\mu) = \sum_{n} \overline{L}_{n}^{s}(\tau,\mu) \text{ with } \overline{L}_{n}^{s}(\tau,\mu) = \begin{pmatrix} I_{n}^{s}(\tau,\mu) \\ Q_{n}^{s}(\tau,\mu) \\ U_{n}^{s}(\tau,\mu) \end{pmatrix} \tag{3}$$

Finally, OSOAA provides the radiance field for the azimuth angle ϕ by applying equation (2).

4.2 Radiative properties of particles

The radiative properties of particles depend on their size distributions and refractive indices (related to their chemical constitution).

Starting with a description of the size distributions supported by OSOAA to model aerosols and hydrosols, this chapter presents the calculations performed by the software to simulate the radiative properties of particles which are required to solve the radiative transfer equation (single scattering albedo, matrix phase function). Some inner mathematical processes are also presented, such as the phase function truncation.

4.2.1 Particle size distributions

The size distribution of aerosols and hydrosols is defined by a function N(r). The value N(r).dr is the number of particles with a radius between [r, r+dr] by unit volume (in μm^{-3}).

4.2.1.1 Aerosol model definition

The aerosol size distribution can be modelled by mono-modal or multi-modal models.

- **Junge's law model**:

$$\boxed{\begin{cases} r \le r_{min} : N_{aer}^{Junge}(r) = r_{rmin}^{-\upsilon} \\ r_{min} < r \le r_{max} : N_{aer}^{Junge}(r) = r^{-\upsilon} \\ r > r_{max} : N_{aer}^{Junge}(r) = 0 \end{cases}} \qquad (4)$$

with

- r_{min} : the minimal radius of aerosols (µm).
  → defined by the user : **AER.MMD.JD.rmin**.
- r_{max} : the maximal radius of aerosols (µm).
  → defined by the user : **AER.MMD.JD.rmax**.
  → or, default and recommended value: 50 µm, CTE_DEFAULT_AER_JUNGE_RMAX in the OSOAA.h file.
- υ : the slope of the Junge's law
  → defined by the user : **AER.MMD.JD.slope**.

Notes:

- **Assumption of a constant number of particles for lowest radii:**
  For aerosols, we introduce a constant value for $r \le r_{min}$ rather than for hydrosols we assume there is no particle with a radius lower to r_{min}.
- The **slope υ = 3.0 is a singular value**:
  If this value υ = 3.0 is entered by the user, the OSOAA code must adjust this value by adding ε_{υ} = 0.05 (parameter CTE_JUNGE_SLOPE_COR in OSOAA.h).

- **Log-Normal size Distribution (LND)**:

$$\boxed{N^{LND}(r) = \frac{1}{r.\sigma.\sqrt{2\pi}} \times \exp\left(-\frac{\ln^2(r/r_m)}{2\sigma^2}\right)} \qquad (5)$$

with

  - r_m : the modal radius of the size distribution (µm).

    → defined by the user : **AER.MMD.LNDradius**.

  - σ : the standard deviation of the size distribution (µm).

    → defined by the user : **AER.MMD.LNDvar**.

- The **WMO models**:

  From the elementary components of the WMO (« Dust Like », « Water Soluble », « Oceanic », « Soot »), it is possible to simulate predefined models (**AER.WMO.Model**: continental, maritime, urban) or to simulate a user model defined by mixing the different components (**AER.WMO.DL**, **AER.WMO.WS**, **AER.WMO.OC**, **AER.WMO.SO**: ratios between 0 and 1)

- The **Shettle & Fenn models**:

  The Shettle & Fenn models allow simulating standard aerosol models (**AER.SF.Model**: tropospheric, urban, maritime or coastal) which take into account the sensitivity of the size distribution and refractive index to the relative air humidity (**AER.SF.RH** in percents).

  These predefined models are based on a mixture of elementary components (Small rural, large rural, small urban, large urban, oceanic particles).

- The **bimodal Log-Normal models**:

  The bimodal Log-Normal distributions simulate aerosol models composed of two kinds of different particles: different chemical composition (refractive indexes) and different size distributions (modelled by LND). They distinguish a coarse and a fine modes of particles.

  The volume size distribution of bimodal models is given by:

$$\frac{dV(r)}{d\ln r} = \sum_{i=1}^{2} \frac{C_{V,i}}{\sigma_i \sqrt{2\pi}} \times \exp\left[\frac{-\ln^2(r/r_i)}{2\sigma_i^2}\right] \qquad (6)$$

with :

  - $C_{V,i}$: the volume concentration for mode i particles (in µm³ / µm²).

    → defined by the user: **AER.BMD.CoarseVC** for the coarse mode and **AER.BMD.FineVC** for the fine mode, in case of using a user definition of the volume concentrations (**AER.BMD.VCdef** = 1).

- r_i: the modal radius of the mode i LND (in µm).

  → defined by the user: **AER.BMD.CM.SDradius** for the coarse mode and **AER.BMD.FM.SDradius** for the fine mode.

- σ_i: the standard deviation of the mode i LND.

  → defined by the user: **AER.BMD.CM.SDvar** for the coarse mode and **AER.BMD.FM.SDvar** for the fine mode.

The ratio of "coarse mode" and "fine mode" can be defined in two ways:

- The coefficients are provided by the user (volume concentration for each mode of particles): option **AER.BMD.VCdef** = 1.

- The coefficients are estimated from the ratio of the coarse mode optical thickness on the total aerosol optical thickness (combining the two modes): **AER.BMD.VCdef** = 2.

$$r(\lambda_{ref}) = \frac{\tau_{aer}^{C}(\lambda_{ref})}{\tau_{aer}^{tot}(\lambda_{ref})} \tag{7}$$

→ defined by the user: **AER.BMD.RAOT**.

with $\tau_{aer}^{tot}(\lambda_{ref}) = \tau_{aer}^{F}(\lambda_{ref}) + \tau_{aer}^{C}(\lambda_{ref})$ for λ_{ref} the reference wavelength for the aerosol optical thickness.

From the size distribution and refractive index of each mode, OSOAA calculates the fine and coarse scattering cross-sections ($\tilde{\sigma}_{sca}^{F}(\lambda_{ref})$, $\tilde{\sigma}_{sca}^{C}(\lambda_{ref})$) and extinction cross-sections ($\tilde{\sigma}_{ext}^{F}(\lambda_{ref})$, $\tilde{\sigma}_{ext}^{C}(\lambda_{ref})$), as explained in section 4.2.2.

Then, it calculates

$$\begin{cases} C_{V,C} = \dfrac{r(\lambda_{ref}) \times \tau_{aer}^{tot}(\lambda_{ref})}{\tilde{\sigma}_{ext}^{C}(\lambda_{ref})} \\ \\ C_{V,F} = \dfrac{(1 - r(\lambda_{ref})) \times \tau_{aer}^{tot}(\lambda_{ref})}{\tilde{\sigma}_{ext}^{F}(\lambda_{ref})} \end{cases} \tag{8}$$

Finally, these coefficients are normalized:

$$\alpha_F = \frac{C_{V,F}}{C_{V,F} + C_{V,C}} \quad \text{and} \quad \alpha_C = \frac{C_{V,C}}{C_{V,F} + C_{V,C}} \tag{9}$$

4.2.1.2 Hydrosol model definition

The size distribution of scattering particles in the sea water (mineral-like particles or phytoplankton) is modelled by a main mode following a Junge's law model and optional secondary and tertiary modes following Log-Normal distributions.

Each mode is characterized by a refractive index and its own size distribution parameters.

- **Junge's law model**: Main mode

$$\boxed{\begin{cases} r \le r_{min} : N_{hyd}^{Junge}(r) = r_{rmin}^{-\upsilon} \\ r_{min} < r \le r_{max} : N_{hyd}^{Junge}(r) = r^{-\upsilon} \\ r > r_{max} : N_{hyd}^{Junge}(r) = 0 \end{cases}} \qquad (10)$$

with

- r_{min} : the minimal radius of hydrosols (µm).
  → defined by the user : **PHYTO.JD.rmin**.
  → or, default and recommended value: 0.01 µm
  (CTE_DEFAULT_HYD_JUNGE_RMIN in the OSOAA.h file)

- r_{max} : the maximal radius of hydrosols (µm).
  → defined by the user : **PHYTO.JD.rmax**.
  → or, default and recommended value: 200 µm,
  (CTE_DEFAULT_HYD_JUNGE_RMAX in the OSOAA.h file).

- υ : the slope of the Junge's law
  → defined by the user : **HYD.MMD.JD.slope**.

Notes:

- **Assumption of a constant number of particles for lowest radii:**

  For aerosols, we introduce a constant value for $r \le r_{min}$ rather than for hydrosols we assume there is no particle with a radius lower than r_{min}. Indeed, it is well known that the number of hydrosols decreases for smallest particles. But, as it cannot be measured, it is better to assume the number of very small particles is null, as the scattering tends toward the molecular scattering case.

- The **slope υ = 3.0 is a singular value**:

  If this value υ = 3.0 is entered by the user, the OSOAA code must adjust this value by adding ε_υ = 0.05 (parameter CTE_JUNGE_SLOPE_COR in OSOAA.h).

- **Log-Normal size Distribution (LND)**: secondary and tertiary modes (optional)

$$\boxed{N_i^{LND}(r) = \frac{1}{r.\sigma_i.\sqrt{2\pi}} \times \exp\left[\frac{-\ln^2(r/r_i)}{2\sigma_i^2}\right]} \qquad (11)$$

with

- r_i : the modal radius of the size distribution for mode i (µm).

  → defined by the user : **PHYTO.LND.SM.SDradius** and **PHYTO.LND.TM.SDradius**, respectively for the secondary and tertiary modes.

- σ_i : the standard deviation of the size distribution for mode i.

  → defined by the user : **PHYTO.LND.SM.SDvar** and **PHYTO.LND.TM.SDvar**, respectively for the secondary and tertiary modes.

The relative ratio of the modes is given by:

$$\boxed{N(r) = \alpha_1^{Junge} \times N_1^{Junge}(r) + \sum_{C=2}^{3} \alpha_i^{LND} \times N_i^{LND}(r)} \qquad (12)$$

with $\alpha_i = N_i / N_{tot}$: the relative number of particles for the mode i, expressed as the ratio between the number of particles of the mode i and the total number of particles.

These rates are provides by the user (**PHYTO.JD.rate**, **PHYTO.LND.SM.rate**, **PHYTO.LND.TM.rate** for the phytoplankton; **SED.JD.rate**, **SED.LND.SM.rate**, **SED.LND.TM.rate** for the Mineral-Like particles).

They respect: $$\boxed{\sum_{C=1}^{Nb\ Modes} \alpha_C = 1} \qquad (13)$$

4.2.2 Phase function matrices and cross sections calculation

Let's note $\tilde{L}_\lambda(\tau,\mu',\phi') = \begin{pmatrix} I_\lambda(\tau,\mu',\phi') \\ Q_\lambda(\tau,\mu',\phi') \\ U_\lambda(\tau,\mu',\phi') \end{pmatrix}$ an incident beam toward the direction (µ', ϕ') at the optical depth τ, expressed as a Stokes' vector.

The scattering of $\tilde{L}_\lambda(\tau,\mu',\phi')$ to the direction (µ, ϕ) is given by :

$$d\tilde{L}_\lambda(\tau,\mu,\phi) = \frac{\omega_\lambda(\tau)}{4\pi}.\tilde{\tilde{P}}_\lambda(\tau,\mu,\phi,\mu',\phi').\tilde{L}_\lambda(\tau,\mu',\phi').\frac{d\tau}{\mu} \qquad (14)$$

- The single scattering albedo, $\omega_\lambda(\tau)$, is informative on the ratio of scattered energy.

  It is related to the scattering and extinction cross-sections by:

$$\omega_\lambda(\tau) = \frac{\tilde{\sigma}_{sca}^{\lambda}(\tau)}{\tilde{\sigma}_{ext}^{\lambda}(\tau)} \quad (15)$$

- The phase matrix, $\tilde{\tilde{P}}_\lambda(\tau,\mu,\phi,\mu',\phi')$, is informative on the spatial distribution of the scattered light, for intensity and polarization. For a frame linked to the scattering plane, it can be expressed by:

$$\tilde{\tilde{P}}_\lambda(\Theta) = \begin{pmatrix} P_{11}(\Theta) & P_{12}(\Theta) & 0 \\ P_{12}(\Theta) & P_{22}(\Theta) & 0 \\ 0 & 0 & P_{33}(\Theta) \end{pmatrix} \quad (16)$$

  applied to the Stokes' parameters (I, Q, U), where $P_{11}(\Theta)$ is the intensity phase function and other terms are related to the polarization.

  Note: For spherical particles $P_{22} = P_{11}$.

These radiative parameters must be calculated for each component ***c*** of the environment ($\tilde{\sigma}_{sca}^{(c)}$, $\tilde{\sigma}_{ext}^{(c)}$ and $P_c(\Theta)$), in order to be able to estimate its global scattering properties.

They are considered constant throughout the atmospheric and maritime profiles, but their amounts (related to their optical thicknesses) vary with the different layers of the profiles.

4.2.2.1 Radiative properties of an individual component

Inner calculations of OSOAA assume particles are spherical, which allows applying the Mie theory [DR10] to compute the radiative properties of a component.

Each component of the environment is defined by its chemical constitution (refractive index) and size distribution.

The refractive index of a component is : $m = m_r + i \times m_i$ (where $m_i < 0$ is related to the particle absorption).

The Mie theory allows calculating the radiative properties of a spherical particle, for a given refractive index m, as a function of the size parameter $\alpha = 2\pi r/\lambda$, where r is the particle radius and λ is the wavelength of the incident light:

- the Mie extinction efficiency factor : $Q_{ext}(m, \alpha)$,
- the Mie scattering efficiency factor : $Q_{sca}(m, \alpha)$,

- the Mie phase functions versus the scattering angle Θ :

$$\tilde{\tilde{P}}_{mie}(\Theta,m,\alpha)=\begin{pmatrix} P_{mie}(\Theta,m,\alpha) & Q_{mie}(\Theta,m,\alpha) & 0 \\ Q_{mie}(\Theta,m,\alpha) & P_{mie}(\Theta,m,\alpha) & 0 \\ 0 & 0 & T_{mie}(\Theta,m,\alpha) \end{pmatrix} \qquad (17)$$

OSOAA computes these coefficients and functions for a set of values of the size parameter α :

$$\begin{array}{llll} \alpha \le 0{,}1 & \Rightarrow \Delta\alpha = 0{,}0001 & 10 < \alpha \le 30 & \Rightarrow \Delta\alpha = 0{,}05 \\ 0{,}1 < \alpha \le 1{,}0 & \Rightarrow \Delta\alpha = 0{,}001 & 30 < \alpha \le 100 & \Rightarrow \Delta\alpha = 0{,}1 \\ 1{,}0 < \alpha \le 10 & \Rightarrow \Delta\alpha = 0{,}01 & 100 < \alpha & \Rightarrow \Delta\alpha = 1{,}0 \end{array}$$

Accounting for the size distribution of the component, **N(r)**, and for a given wavelength, λ, we can estimate from Mie computations:

- The extinction coefficient (in μm^{-1}) and the extinction cross section (in μm^2) :

$$\boxed{\sigma_{ext}(\lambda)=\int_{r=0}^{\infty}\pi.r^2.Q_{ext}(m,r,\lambda).N(r).dr}$$

$$\text{and} \quad \boxed{\tilde{\sigma}_{ext}(\lambda)=\sigma_{ext}(\lambda)\Big/\int_{r=0}^{\infty}N(r).dr} \qquad (18.a)$$

- The scattering coefficient (in μm^{-1}) and the scattering cross section (in μm^2)

$$\boxed{\sigma_{sca}(\lambda)=\int_{r=0}^{\infty}\pi.r^2.Q_{sca}(m,r,\lambda).N(r).dr}$$

$$\text{and} \quad \boxed{\tilde{\sigma}_{sca}(\lambda)=\sigma_{sca}(\lambda)\Big/\int_{r=0}^{\infty}N(r).dr} \qquad (18.b)$$

♦ N(r).dr is the number of particles with a radius between [r, r+dr] by volume (in μm^{-3}).

♦ $\pi.r^2.Q_e(m, \alpha)$ is the extinction cross section for a particle of radius r and for the wavelength λ (in μm^2).

- We then derive the single scattering albedo by:

$$\boxed{\omega_0(\lambda)=\frac{\sigma_{sca}(\lambda)}{\sigma_{ext}(\lambda)}} \qquad (19)$$

- We also calculate the functions of the phase matrix, expressed for the scattering plane as a reference plane for the frame:

$$P_{11}(\lambda,\Theta)=\frac{1}{\sigma_{sca}(\lambda)}\times\int_{r=0}^{\infty}\pi.r^2.Q_{sca}(m,r,\lambda).P_{mie}(\Theta,m,r,\lambda).N(r).dr \qquad (20.a)$$

$$P_{12}(\lambda,\Theta)=\frac{1}{\sigma_{sca}(\lambda)}\times\int_{r=0}^{\infty}\pi.r^2.Q_{sca}(m,r,\lambda).Q_{mie}(\Theta,m,r,\lambda).N(r).dr \qquad (20.b)$$

$$P_{33}(\lambda,\Theta)=\frac{1}{\sigma_{sca}(\lambda)}\times\int_{r=0}^{\infty}\pi.r^2.Q_{sca}(m,r,\lambda).T_{mie}(\Theta,m,r,\lambda).N(r).dr \qquad (20.c)$$

The probability for a scattering toward the scattering angle Θ, into the solid angle $d\Omega$, is given by $P_{11}(\Theta).d\Omega$ / 4π.

The phase function is normalized in order to get: $\iint_{Space} P_{11}(\Theta).d\Omega / 4\pi = 1$

4.2.2.2 Radiative properties of a particle mixture

Let's consider an element of volume including N particles of different components.

We note N_c the number of particles for the component c and define the coefficient α_c by:

$$N_c = \alpha_c \times N \qquad (21)$$

The radiative properties of each elementary component are:

- the extinction and scattering cross-sections $\tilde{\sigma}_{ext}^{(c)}$ and $\tilde{\sigma}_{sca}^{(c)}$.
- the phase matrix $P_c(\Theta)$ of the size distribution c.

The radiative properties of the mixture can be calculated from the radiative properties of the elementary components and from coefficients α_c:

- **Single scattering albedo of the mixture:**

The extinction and scattering cross-sections $\tilde{\sigma}_{ext}$ and $\tilde{\sigma}_{sca}$ are:

$$\begin{cases} N\times\tilde{\sigma}_{sca} = \sum_c N_c \times \tilde{\sigma}_{sca}^{(c)} \\ N\times\tilde{\sigma}_{ext} = \sum_c N_c \times \tilde{\sigma}_{ext}^{(c)} \end{cases} \qquad (22)$$

Then, the single scattering albedo is:

$$\omega_0 = \frac{N \times \tilde{\sigma}_{sca}}{N \times \tilde{\sigma}_{ext}} = \frac{\sum_c N_c \times \tilde{\sigma}_{sca}^{(c)}}{\sum_c N_c \times \tilde{\sigma}_{ext}^{(c)}} \tag{23}$$

$$\text{also: } \boxed{\omega_0 = \frac{\sum_c \alpha_c \times \tilde{\sigma}_{sca}^{(c)}}{\sum_c \alpha_c \times \tilde{\sigma}_{ext}^{(c)}}} \tag{24}$$

- **Phase matrix of the mixture:**

The phase function of the mixture is given by:

$$N \times \tilde{\sigma}_{sca} \times p_{11}(\Theta) = \sum_c N_c \times \tilde{\sigma}_{sca}^{(c)} \times p_{11}^{(c)}(\Theta) \tag{25}$$

$$\text{also: } \boxed{p_{11}(\Theta) = \frac{\sum_c \alpha_c \times \tilde{\sigma}_{sca}^{(c)} \times p_{11}^{(c)}(\Theta)}{\sum_c \alpha_c \times \tilde{\sigma}_{sca}^{(c)}}} \tag{26}$$

There is a similar relation for functions $P_{22}(\Theta)$ and $P_{33}(\Theta)$ of the phase matrix.

For numerical purpose, it is convenient to expand the phase functions into Legendre functions. Then, OSOAA finally expresses the matrix phase functions by a set of coefficients, α_k, β_k, γ_k, δ_k and ξ_k, from expansions into generalized Legendre functions. [DR9].

- **Refractive index of the mixture:**

$$\boxed{\langle m_r \rangle = \sum_{c=1,3} \alpha_c \times m_{r,c}} \tag{27}$$

From an empirical approach, we estimate the mean refractive index of a particle mixture by weighting the refractive index of each component by its relative amount of particles.

This estimate is useful to calculate the scattering coefficient profile of Mineral-Like particles (see §4.3.3.4).

4.2.3 Phase function truncation

For large particles, the forward peak of the phase function can be very strong, in a cone of a few degrees aperture. In order to reduce the expansion of the phase function and perform faster simulations, a phase function truncation can be applied.

As this phase function truncation changes the spatial distribution of the scattered energy, in the forward direction, the other radiative parameters must be adjusted in order to preserve the consistency of the radiative transfer calculation.

By default, the truncation procedure is applied for aerosols and for marine particles (phytoplankton and Mineral-Like particles). It can sometimes be cancelled for aerosols but not for marine particles which are always large particles.

For numerical computations, the phase function expansion in the frame of Legendre functions can be limited to a maximal order L which depends on the kind of scattering matter:

- For **molecular scattering**, L = 2.
- For **aerosols or hydrosols scattering**, L is selected by a threshold ε for which $\beta_{L+1} < \varepsilon$. This can lead to a very high expansion order in case of large particles for which the phase function presents a strong forward peak. In order to reduce the maximal order L, we can consider that the energy scattered toward the forward direction is simply transmitted. This is equivalent to reduce the phase function forward peak.

Let's call Θ_1 and Θ_2 the scattering angles for which a delta approximation of the phase function is applied. By default, OSOAA uses $\cos \Theta_1 = 0.8$ ($\Theta_1 \approx 37°$) and $\cos \Theta_2 = 0.94$ ($\Theta_2 \approx 20°$), parameters CTE_AER_MU1_TRONCA and CTE_AER_MU2_TRONCA in the OSOAA.h file. The phase function is truncated for angles $\Theta < \Theta_2$ by the function:

$$\log[p_{tr}(\Theta)] = AA \times \Theta + B \tag{28}$$

$$\text{with} \quad \begin{cases} AA = \dfrac{\log[p(\Theta_2)] - \log[p(\Theta_1)]}{\Theta_2 - \Theta_1} \\ B = \dfrac{\Theta_2 \times \log[p(\Theta_1)] - \Theta_1 \times \log[p(\Theta_2)]}{\Theta_2 - \Theta_1} \end{cases} \tag{29}$$

Therefore, the truncated phase function is:

$$\boxed{\begin{cases} \text{Si } \Theta < \Theta_2 \Rightarrow p_{tr}(\Theta) = 10^{\log[p(\Theta_2)] + \frac{\Theta - \Theta_2}{\Theta_2 - \Theta_1} \times (\log[p(\Theta_2)] - \log[p(\Theta_1)])} \\ \text{Si } \Theta \geq \Theta_2 \Rightarrow p_{tr}(\Theta) = p(\Theta) \end{cases}} \tag{30}$$

The polarized phase functions are adjusted by the following relation:

$$\boxed{\begin{cases} P_{12\,tr}(\Theta) = P_{12}(\Theta) \times [P_{tr}(\Theta)/P(\Theta)] \\ P_{33\,tr}(\Theta) = P_{33}(\Theta) \times [P_{tr}(\Theta)/P(\Theta)] \end{cases}} \qquad (31)$$

The coefficients associated to the phase matrix expansion [α(k), β(k), δ(k), γ(k) and ξ(k)] are then calculated from these truncated functions.

The optical thickness and single scattering albedo of the atmospheric and marine layers must be adjusted in order to unchange the global radiative properties by using the truncated phase functions.

The truncation coefficient F gives the ratio of energy which is not scattered when applying the phase function truncation:

$$\boxed{F = \iint_{\text{espace}} [p(\Theta) - p_{tr}(\Theta)] . \frac{d\omega}{4\pi}} \quad \text{also: } \boxed{F = \frac{1}{2} \times \int_0^{\pi} [p(\Theta) - p_{tr}(\Theta)] . \sin\Theta . d\Theta} \qquad (32)$$

with p(Θ) the original normalized phase function and $p_{tr}(\Theta)$ the truncated one.

We get:

- The extinction optical thickness, adjusted to the phase function truncation:

$$\boxed{\tau_{ext}^{tr} = \tau_{ext} \times (1 - \omega_0 . F)} \qquad (33.a)$$

- The scattering optical thickness, adjusted to the phase function truncation:

$$\boxed{\tau_{sca}^{tr} = \tau_{ext}^{tr} \times \omega_0^{tr}} \qquad (33.b)$$

or also: $$\boxed{\tau_{sca}^{tr} = \tau_{sca} \times (1 - F)} \qquad (33.c)$$

Note: A similar formulation is available for the scattering coefficient σ_{sca}^{tr} (also called b^{tr} in the marine environment):

$$\boxed{\sigma_{sca}^{tr} = \sigma_{sca} \times (1 - F)} \qquad (33.d)$$

- The single scattering albedo, adjusted to the phase function truncation:

$$\boxed{\omega_0^{tr} = \omega_0 \times \left(\frac{1 - F}{1 - \omega_0 . F} \right)} \qquad (33.e)$$

- The truncated and normalized phase functions:
- $$\begin{cases} P_{tr}^{norma}(\Theta) = \dfrac{P_{tr}(\Theta)}{1-F} \\ P_{12\,tr}^{norma}(\Theta) = \dfrac{P_{12\,tr}(\Theta)}{1-F} \\ P_{33\,tr}^{norma}(\Theta) = \dfrac{P_{33\,tr}(\Theta)}{1-F} \end{cases} \qquad (33.f)$$

The coefficients β_k of the expansion into Legendre polynomials (for a maximal order of the development L) become β_k^{tr} with $\beta_k = (2k+1).F + (1-F).\beta_k^{tr}$ (for a maximal order L* < L).

4.3 Atmosphere and sea profiles definition

The atmospheric and marine vertical profiles describe the evolving of the extinction optical thickness from TOA to the bottom of sea. They also provide the mixing rate of components located in the environment.

This chapter presents the methods applied by OSOAA to define these profiles.

4.3.1 Atmospheric and marine profiles description

The atmospheric and marine profiles are not generated versus the altitude or depth but versus the optical thickness, which is much more convenient for radiative transfer calculations (Figure 4). The stronger absorption in the sea requires a higher number of levels for the discretization of the sea vertical profile (CTE_NT_SEA in the OSOAA.h file, called NT_{sea} below) than for the atmospheric one (NT_{atm}, CTE_NT_ATM in OSOAA.h).

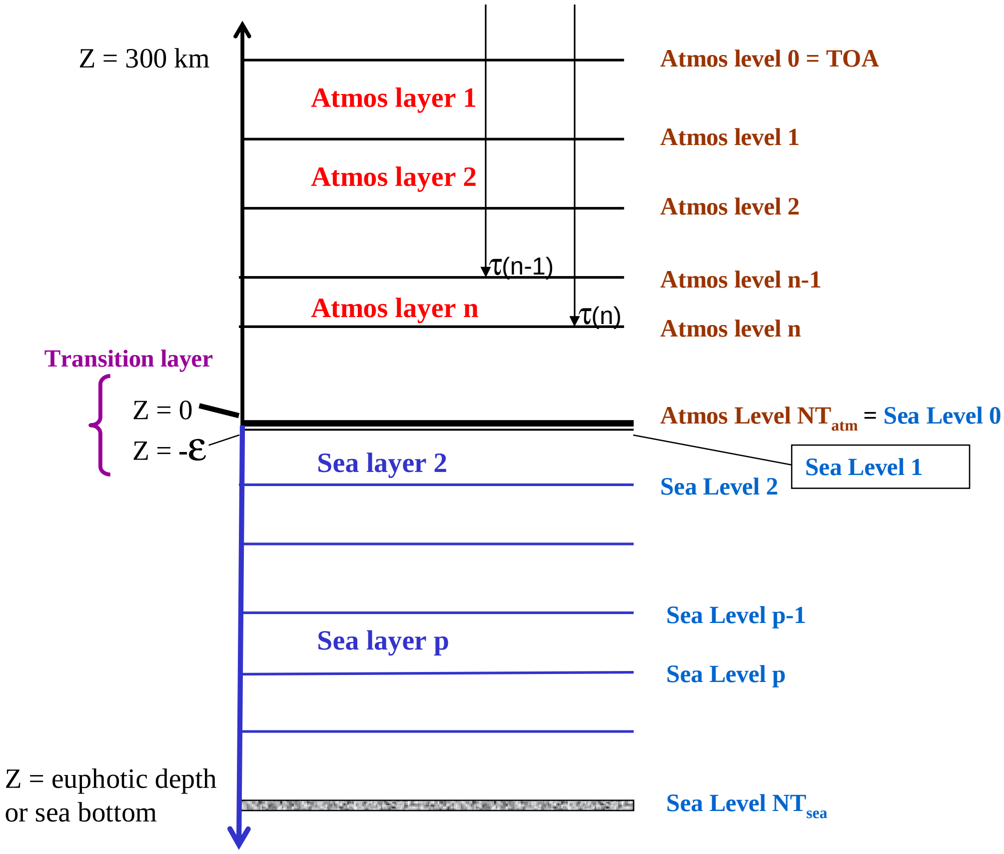


Figure 4 : Atmosphere and sea profiles discretization

From the optical thickness of each component for each level, OSOAA calculates the mixing rate of components in each layer n (between levels n-1 and n) in term of scattering contribution in the layer.

This information is used by OSOAA to calculate the global phase function of each layer. Indeed, from the scattering mixing rate and the phase matrix of each component, the overall phase matrix can be expressed by:

$$\boxed{\omega_0(\tau)\times \tilde{\tilde{P}}(\tau,\Theta)=\sum_{i=1}^{N} pc(i,\tau)\times \tilde{\tilde{P}}_i(\Theta)} \qquad (34)$$

with

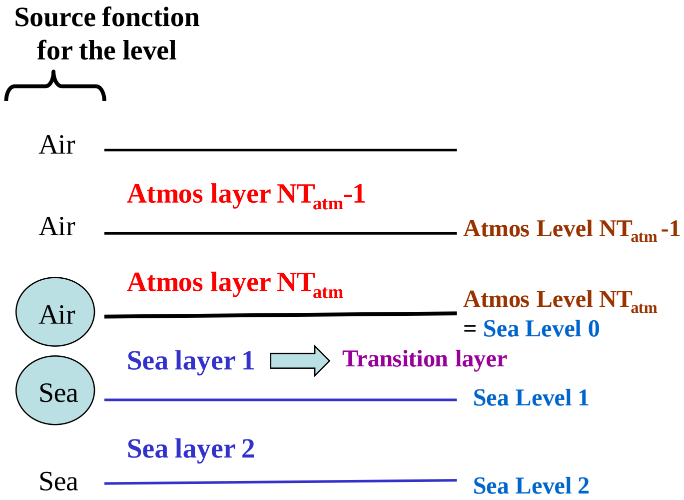
- $\omega_0(\tau)$: the overall single scattering albedo at the level of optical thickness τ
- $pc(i,\tau)$: the contribution of the component *i* to the scattering for the optical thickness τ (scattering mixing rate of component i)

  Note: the single scattering albedo of each components is included in $pc(i,\tau)$ as it expresses a mixing rate related to the scattering.
- $\tilde{\tilde{P}}_i(\Theta)$: the phase matrix of the component *i* (which is assumed to be independent of the optical thickness)

For each level n, the phase function characterises the scattering properties of the layer n just above.

Notes:

- The atmospheric components simulated by OSOAA are molecules and aerosols. OSOAA does not take into account the gaseous absorption.
- A fine transition layer is defined as the first layer of the sea profile (i.e., entrance of the light into the ocean).



It allows avoiding numerical troubles on the vertical integration of radiance due to the environment change (because of the quick variation of the scattering source functions between the last atmospheric level and the first maritime one, as shown on Figure 5).

The optical thickness of this transition layer is defined by CTE_TRANS_OPT_THICKNESS (parameter in the OSOAA.h file).

Figure 5 : Transition layer between atmosphere and sea

4.3.2 Atmospheric optical thickness profile

The molecular scattering depends on the atmospheric pressure profile and the wavelength. The profile of pressure is modelled by an exponential decrease versus the altitude, characterized by the height scale h_{mol} (**–AP.HR**, in km, typically 8 km). The molecular optical thickness for a given altitude z and for the wavelength λ of radiance simulation, is then:

$$\boxed{\tau_{mol}(z) = \tau_{mol}^{surf} \times \exp(-z / h_{mol})} \qquad (35)$$

The molecular optical thickness at ground level τ_{mol}^{surf} is provided by the user (**–AP.MOT**) or calculated from the atmospheric pressure (**–AP.Pressure)** by the Hansen & Travis formulation [DR7]:

$$\boxed{\tau_{mol}^{surf} = \frac{P}{P_0} \times \left(\frac{84,35}{\lambda^4} + \frac{-1,225}{\lambda^5} + \frac{1,4}{\lambda^6} \right) \times 10^{-4}} \qquad (36)$$

where

- λ is the wavelength (in µm) **–OSOAA.Wa**
- P is the atmospheric pressure (in mb) **–AP.Pressure**
- P_0 is the standard atmospheric pressure (parameter CTE_STD_PRESSURE in the OSOAA.h file: 1013 mb).

The aerosol optical thickness profile is defined following the same model:

$$\boxed{\tau_{aer}(\lambda, z) = \tau_{aer}^{surf}(\lambda) \times \exp(-z / h_{aer})} \qquad (37)$$

where

- h_{aer} is the aerosol scale height (in km) **–AP.HA**
- $\tau_{aer}^{surf}(\lambda)$ is the total aerosol optical thickness for the wavelength λ (defined for the radiance simulation).

  This AOT is calculated from the reference AOT $\tau_{aer}^{surf}(\lambda_{ref})$, defined by the user (**AER.AOTref**) for a reference wavelength λ_{ref} (**AER.Waref**), by using the ratio of the extinction coefficients for these two wavelengths:

  $$\boxed{\tau_{aer}^{surf}(\lambda) = \tau_{aer}^{surf}(\lambda_{ref}) \times \frac{\tilde{\sigma}_{aer}^{ext}(\lambda)}{\tilde{\sigma}_{aer}^{ext}(\lambda_{ref})}} \qquad (38)$$

  The extinction coefficients are calculated from the aerosol model parameters.

OSOAA calculates both the profile of the total extinction optical thickness and the profile of scattering mixing rate for molecules and aerosols. The file content and format are presented in section §3.4.3 (page 61).

The **total extinction optical thickness** for each atmospheric level p is:

$$\boxed{\tau_{tot}(p) = \tau_{mol}\left[z(p)\right] + \tau_{aer}\left[z(p)\right]} \tag{39}$$

by cumulating the optical thickness of molecules and aerosols.

The **scattering mixing rate of the molecules and aerosols** for each level p is:

$$\boxed{\begin{cases} pc_{sca}^{ray}(p) = \dfrac{\tau_{mol}\left[z(p)\right]/h_{mol}}{\tau_{mol}\left[z(p)\right]/h_{mol} + \tau_{aer}\left[z(p)\right]/h_{aer}} \\ \\ pc_{sca}^{aer}(p) = \dfrac{\omega_0^{aer} \times \tau_{aer}\left[z(p)\right]/h_{aer}}{\tau_{mol}\left[z(p)\right]/h_{mol} + \tau_{aer}\left[z(p)\right]/h_{aer}} \end{cases}} \tag{40}$$

These mixing rates are used to calculate the mixture-averaged phase function, according to equation (34).

Note: OSOAA does not take into account for atmospheric gaseous absorption, but it simulates the aerosol absorption (relying on the imaginary part of their refractive index).

4.3.3 Marine optical thickness profile

Scattering and absorption in the sea water are due to many contributors: the water molecules, phytoplankton, mineral-like particles, yellow substance and detritus (dead phytoplankton particles).

As for the atmosphere, the radiative characterization of the marine environment is provided by its single scattering albedo and its phase function (including the polarization) throughout the optical thickness profile. Hydrosols (phytoplankton and mineral-like particles) can be modelled by a size distribution and a refractive index correlated to their chemical composition. OSOAA also can use experimental phase function measurements and scattering coefficients of hydrosols.

4.3.3.1 Sea depth

The user can define the sea depth (**-Sea.Depth**, in meters).

If it is not defined by the user, the euphotic depth will be used from Morel tabulated data correlated to the chlorophyll concentration at sea surface (Table 11): CTE_FIC_EUPH_DEPTH file defined in OSOAA.h.

Table 11 : Relationship between the euphotic depth and the chlorophyll concentration at sea surface for case 1 waters (Morel, 1988 [DR12])

Chl (mg.m-3)	Zeu (m)
0.00	183.0
0.01	153.0
0.03	129.0
0.05	115.0
0.10	95.0
0.20	75.0
0.30	64.0
0.50	52.0
1.00	39.0
2.00	29.0
3.00	24.0
5.00	19.0
10.00	14.0
20.00	10.0
30.00	8.0

The euphotic depth is estimated from the surface concentration of chlorophyll, by using tabulated data available for case 1 sea waters (Morel, 1988 [DR12]).

The provided file (OSOAA_SEA_EUPH_DEPTH.txt) is located in the repertory `${OSOAA_ROOT}`/fic. It is defined by the parameter CTE_FIC_EUPH_DEPTH. Its contents are presented in Table 11.

A linearly interpolation is applied to get the euphotic depth corresponding to the user's defined value of the chlorophyll concentration at sea surface (**PHYTO.Chl**)

Note: A maximal value of the sea optical thickness, at the wavelength for radiance simulation, is defined by the parameter CTE_SEA_T_LIMIT (defined in OSOAA.h). If the optical thickness for the sea depth is higher than this threshold, the sea optical thickness profile is calculated till its limit value (30 is suggested).

4.3.3.2 Sea molecule profile

The **sea molecular scattering coefficient** is calculated by the Morel's model (1974) [DR11] :

$$\boxed{b_w(\lambda) = 0{,}00288 \times \left(\frac{\lambda}{500}\right)^{-4{,}32}} \qquad (41)$$

The **sea molecular absorption coefficient** is calculated by OSOAA from tabulated data between 200 nm to 2449 nm: CTE_FIC_MOL_SPECTRAL_DATA file defined in OSOAA.h (see Figure 6):

- Pope & Fry (1997) data from 380 to 730 nm [DR13],
- Kou et al. (1993) data from 730 to 2449 nm [DR8]
- Smith & Baker (1981) data for wavelengths lower to 380 nm and for wavelengths higher than 730 nm [DR15].

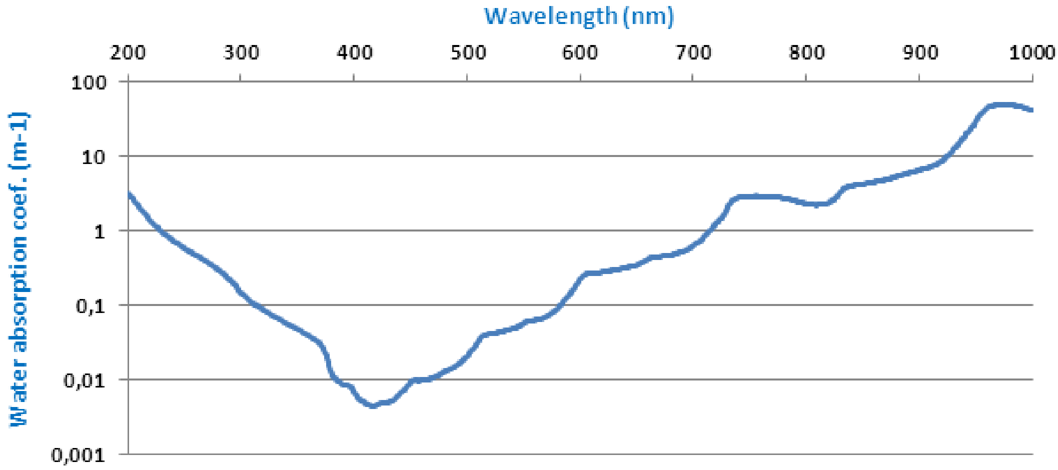


Figure 6 : Tabulated molecular absorption coefficients from 200 to 1000 nm.

For the wavelength of the radiance simulation (**OSOAA.Wa**) the absorption coefficient is linearly interpolated from tabulated values.

As the puresea water density is considered as a constant value from the sea bottom to the surface, the molecular scattering and absorption coefficients are constant throughout the sea profile.

Notes:

- The CTE_FIC_MOL_SPECTRAL_DATA file also provides sea molecular scattering coefficients. These values are not used by the OSOAA code but are close to values calculated by the used relation (41).

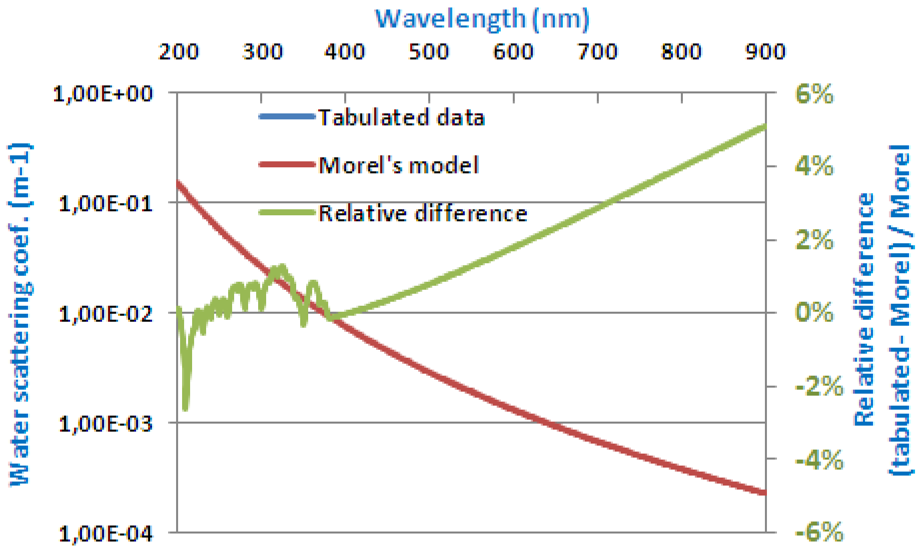


Figure 7 : Comparison of tabulated molecular scattering coefficients and values modelled by MOREL (1974) from 200 to 900 nm. Relative difference plotted in green line (see right scale).

- The user cannot perform a simulation under the minimal wavelength CTE_WAMIN (defined in the OSOAA.h file) and over the maximal tabulated wavelength.

4.3.3.3 Chlorophyll profile

The profile of chlorophyll concentration Chl(z), for z the sea depth in meters, can be modelled by:

- **Case 1** : An **homogeneous profile** (-**PHYTO.ProfilType 1**)

$$\boxed{Chl(z) = C_0} \qquad (42)$$

with C_0 the chlorophyll A concentration at sea surface, defined by the user (**PHYTO.Chl,** in $mg.m^{-3}$)

- **Case 2** : A **Gaussian profile** (-**PHYTO.ProfilType 2**)

$$\boxed{Chl(z) = C_1 + C_0.\exp\left(-\frac{(z - z_{max})^2}{2\sigma^2}\right)} \qquad (43)$$

with the following parameters defined by the user

- C_0 : the chlorophyll A concentration at sea surface (**PHYTO.Chl,** in mg.m^{-3}).
- C_1 : the constant background biomass (**PHYTO.GP.Chlbg,** in mg.m^{-3}).
- Z_{max} : the maximum deep of the Gaussian chlorophyll profile (**PHYTO.GP.Deep**, in m)
- σ : the width of the chlorophyll peak (**PHYTO.GP.Width**, in m)

- **Case 3** : A chlorophyll profile defined by an **userfile** (-**PHYTO.ProfilType 3**)

  The userfile is defined by the parameter **PHYTO.Userfile.**

  This file must provide the chlorophyll concentration for a set of sea depths.

  Format for each line: Z_user Chl_user

  (sea depth in meters, chlorophyll concentration in mg.m^{-3}).

  The maximal number of lines cannot exceed the value of the parameter CTE_NBWA_MAX (defined in the OSOAA.h file).

  The first value Z_user must be 0 (surface) and the last value must exceed the sea depth (provided by the user or the euphotic depth calculated by OSOAA)

Note: the shape of the chlorophyll concentration is not very important because the light scattering that is observed by a satellite applies mainly in the few first meters below the surface.

The phytoplankton profile of scattering and absorption coefficients is derived from the chlorophyll concentration profile Chl(z) (in mg.m^{-3}) by:

Scattering coefficient for the phytoplankton [DR12] :

$$\boxed{\sigma_{sca}^{phyto}(\lambda, z) = 0.30 \times \left(\frac{550}{\lambda}\right) \times \mathrm{Chl}(z)^{0.62}} \tag{44}$$

for λ the simulation wavelength (in nm).

Absorption coefficient for the phytoplankton [DR1] :

$$\boxed{\sigma_{abs}^{phyto}(\lambda, z) = \mathrm{AP}(\lambda) \times \mathrm{Chl}(z)^{\mathrm{EP}(\lambda)}} \tag{45}$$

where the AP(λ) and EP(λ) coefficients are linearly interpolated for the simulation wavelength λ from tabulated data AP(λ_k) and EP(λ_k) defined between 400 and 700 nm (

Table 12 : Coefficients AP(λ) and EP(λ) used to calculate the phytoplankton absorption coefficient (Bricaud et al. 1998, [DR1])

λ (nm)	AP(λ) ($m^2.mg^{-1}$)	EP(λ) (no unit)	λ (nm)	AP(λ) ($m^2.mg^{-1}$)	EP(λ) (no unit)	λ (nm)	AP(λ) ($m^2.mg^{-1}$)	EP(λ) (no unit)
400.	4.3320E-02	0.7026457	500.	2.8819E-02	0.6557435	600.	8.5428E-03	0.8049439
410.	4.6698E-02	0.6881722	510.	2.3181E-02	0.7060035	610.	8.5282E-03	0.8248084
420.	4.9477E-02	0.6711948	520.	1.8943E-02	0.7551307	620.	8.9570E-03	0.8438085
430.	5.1299E-02	0.6542764	530.	1.5987E-02	0.7919776	630.	9.3245E-03	0.8455433
440.	5.2019E-02	0.6349636	540.	1.3722E-02	0.821774	640.	9.7295E-03	0.8373872
450.	4.7932E-02	0.6150956	550.	1.1825E-02	0.8385428	650.	1.0298E-02	0.8142347
460.	4.4552E-02	0.6123579	560.	1.0031E-02	0.8412535	660.	1.3335E-02	0.8229631
470.	4.1530E-02	0.6129361	570.	9.0395E-03	0.8364251	670.	1.9890E-02	0.8177396
480.	3.7741E-02	0.606532	580.	8.8089E-03	0.8276318	680.	1.8300E-02	0.8352283
490.	3.4124E-02	0.6200267	590.	8.9436E-03	0.8117254	690.	8.6832E-03	0.9313893
						700.	3.9341E-03	1.01316

Notes:

- The user cannot perform a simulation under the minimal wavelength CTE_WAMIN (defined in the OSOAA.h file). Its value is correlated to the minimal value of Table 12.
- If the wavelength λ for the simulation is out of the spectral range covered by the file (CTE_FIC_PHYTO_SPECTRAL_DATA) then OSOAA retains AP(λ) = 0 and EP(λ) = 1

4.3.3.4 Mineral-Like Particles profile

The scattering and absorption properties of Mineral-Like particles are highly variable depending on their composition and concentration. Therefore, it does not really exist currently some robust bio-optical models that relate the optical properties and the concentration of these particles.

The Mie theory makes possible the computation of the scattering properties of Mineral-Like particles for a given size distribution and wavelength: phase matrix, scattering cross-section and single scattering albedo calculations.

The scattering and absorption coefficients (in m^{-1}) are correlated to the cross-sections and to the number of particles by unit volume. This number is related to the concentration of particles, to their density and to the volume concentration.

The density of Mineral-Like particles depends on the refractive index of particles (value stored in the file of MLP radiative properties: **MLP.ResFile**, and calculated according to relations 27, defined in section §4.2.2.2, page 80) by:

$$\boxed{d_{sed} = 1000 \times \left(8.036 \times m_r^{sed}(\lambda) - 6.826\right)} \qquad (46)$$

The relative density to water of MLP is : $\dfrac{d_{sed}}{1000\ \mathrm{mg}/\ell}$

d_{sed} is a density in mg.ℓ$^{-1}$ (the pure water one is 1000 mg.ℓ$^{-1}$)

The **scattering coefficient of Mineral-Like particles** ($\sigma_{sca}^{sed}(z)$ in m^{-1}) is given by:

$$\boxed{\sigma_{sca}^{sed}(z) = 10^{-6} \times \frac{C_{sed}(z)}{d_{sed}} \times \frac{\tilde{\sigma}_{sca}^{sed}}{\tilde{V}^{sed}}} \tag{47}$$

with

- C_{sed} (z) : the MLP concentration for the sea depth z (in mg.ℓ$^{-1}$). As the MLP profile is supposed to be homogeneous, the concentration is a constant throughout the profile: $C_{sed}(z) = C_{sed}^{surf}$ (**SED.Csed** defined by the user).
- d_{sed} : the density of Mineral-Like particles (in mg.ℓ$^{-1}$), constant throughout the sea depth,
- $\tilde{V}_{sed}$: the mean volume of particles for the size distribution (in µm3).

$$\boxed{\tilde{V}_{sed} = \frac{4.\pi}{3} \int_{r=0}^{\infty} r^3.n(r).dr \Big/ \int_{r=0}^{\infty} n(r).dr} \tag{48}$$

- $\tilde{\sigma}_{sca}^{sed}$: the scattering cross-section (in µm^2).

$\tilde{V}_{sed}$ et $\tilde{\sigma}_{sca}^{sed}$ are calculated by OSOAA and stored in the « PM_MLP » file resulting from radiative properties calculations. The file content and format are presented in section §3.4.4 (page 63).

The **extinction coefficient of Mineral-Like particles** ($\sigma_{ext}^{sed}(z)$ in m^{-1}) is then given by:

$$\boxed{\sigma_{ext}^{sed}(z) = \frac{\sigma_{sca}^{sed}(z)}{\omega_0^{sed}}} \tag{49}$$

with $\omega_0^{sed} = \tilde{\sigma}_{sca}^{sed} / \tilde{\sigma}_{ext}^{sed}$ the single scattering albedo of MLP, calculated by OSOAA from the cross-sections $\tilde{\sigma}_{ext}^{sed}$ and $\tilde{\sigma}_{sca}^{sed}$ stored in the « PM_MLP » file (see section §3.4.4), resulting from radiative properties calculations.

4.3.3.5 Yellow substance and detritus

The yellow substance and detritus are purely absorbing particles. Their scattering coefficients are null.

The **absorption coefficient of yellow substance (also called Color Dissolved Organic Matter-CDOM**, at the wavelength λ, is derived from the following spectral relation:

$$\boxed{a_{ys}(\lambda) = a_{ys}(440) \times \exp\left[-S^{ys} \times (\lambda - 440)\right]} \tag{50}$$

with

- $a_{ys}(440)$: the absorption coefficient of yellow substance at 440 nm, defined by the user (**YS.Abs440**, in m^{-1}),
- S^{ys} : the coefficient for the spectral variation of the yellow substance absorption for the wavelength of simulation (**YS.Swa**, in m^{-1}).

  Its typical value is included between 0.014 and 0.019 m^{-1} depending on the kind of water. It is a constant value from 350 to 700 nm.

  If it is not defined by the user, a default value is used (parameter CTE_DEFAULT_SPECTRAL_YS in the OSOAA.h file: 0.014 m^{-1}).

The **absorption coefficient of detritus**, at the wavelength λ, is derived from:

$$\boxed{a_{det}(\lambda) = a_{det}(440) \times \exp\left[-S^{det} \times (\lambda - 440)\right]} \tag{51}$$

with

- $a_{det}(440)$: the absorption coefficient of detritus at 440 nm, defined by the user (**DET.Abs440**, in m^{-1}),
- S^{det} : the coefficient for the spectral variation of detritus absorption for the wavelength of simulation (**DET.Swa**, in m^{-1}).

  If it is not defined by the user, a default value is used (parameter CTE_DEFAULT_SPECTRAL_DET in the OSOAA.h file: 0.011 m^{-1}).

The absorbing coefficients of yellow substance and detritus are assumed to be <u>constant throughout the sea profile.</u>

4.3.3.6 Mixture-averaged profile calculations

Radiance calculations are based on the mixture-averaged extinction optical thickness profile in the sea and the mixing rate of components in term of scattering. The file content and format are presented in section §3.4.3 (page 61).

The **total extinction optical thickness** for each depth level p is:

$$\boxed{\tau_{tot}(p) = \tau_{water}(p) + \tau_{phyto}(p) + \tau_{sed}(p) + \tau_{ys}(p) + \tau_{det}(p)} \quad (52)$$

by cumulating the optical thickness of each component (water molecules, phytoplankton, Mineral-Like particles, yellow substance and detritus).

The **scattering mixing rate of the component "comp"** for each depth level p is:

$$\boxed{pc_{sca}^{comp}(p) = \frac{\sigma_{sca}^{comp}(p)}{\sigma_{ext}^{water}(p) + \sigma_{ext}^{phyto}(p) + \sigma_{ext}^{sed}(p) + \sigma_{ext}^{ys}(p) + \sigma_{ext}^{det}(p)}} \quad (53)$$

with:

- $\sigma_{sca}^{comp}(p)$ the scattering coefficient of the component « comp » for the level p.
- $\sigma_{ext}^{comp}(p)$ the extinction coefficient of the component « comp » for the level p (water molecules, phytoplankton, Mineral-Like particles, yellow substance and detritus).

These mixing rates are used to calculate the mixture-averaged phase function in the sea, according to equation (34).

4.3.4 Adjustment of optical thickness profiles to phase function truncation

OSOAA produces the atmospheric profile file (-**PROFILE_ATM.ResFile**) and the marine profile file (-**PROFILE_SEA.ResFile**), which define the optical thickness and the scattering mixing rate of components for each profile level (file content and format in section §3.4.3).

The phase function of aerosols, phytoplankton and mineral-like particles are truncated to replace their peak in the cone of forward scattering by a transmission. Therefore, OSOAA must adjust the data profile to the truncations in order to simulate an equivalent atmosphere and marine environment.

4.3.4.1 Adjustment of the atmospheric profile to the aerosol phase function truncation

OSOAA calculates the atmospheric profile (-**PROFILE_ATM.ResFile**) which provides for each level n:

- $\tau_{ext}(n)$: the extinction optical thickness
- pcaer(n): the mixing rate of aerosols for scattering
- pcray(n): the mixing rate of molecules for scattering

OSOAA also calculates the radiative properties of aerosols (stored in the file -**AER.ResFile**) which include:

- $\omega_0^{aer,tr}$: the aerosol single scattering albedo adjusted to the phase function truncation
- F^{aer} : the truncation coefficient

For the layer n, OSOAA calculates:

- The scattering optical thickness of aerosols:

  Real value: $\Delta\tau_{sca}^{aer}(n) = \Delta\tau_{ext}(n) \times \text{pcaer}(n)$

  Value adjusted to the truncation: $\Delta\tau_{sca}^{aer,tr}(n) = \Delta\tau_{sca}^{aer}(n) \times (1 - F^{aer})$

- The extinction optical thickness of aerosols adjusted to the truncation:

  $$\Delta\tau_{ext}^{aer,tr}(n) = \frac{\Delta\tau_{sca}^{aer,tr}(n)}{\omega_0^{aer,tr}}$$

  The extinction optical thickness of molecules (= the scattering one):

- $\Delta\tau_{ext}^{mol}(n) = \Delta\tau_{ext}(n) \times \text{pcray}(n)$

- The global extinction optical thickness of aerosols adjusted to the truncation:

  $$\tau_{ext}^{tr}(n) = \tau_{ext}^{tr}(n-1) + \Delta\tau_{ext}^{aer,tr}(n) + \Delta\tau_{ext}^{mol}(n)$$

- The scattering mixing rate adjusted to the truncation:

  $$\begin{cases} \text{pcaer}^{tr}(n) = \dfrac{\Delta\tau_{sca}^{aer,tr}(n)}{\Delta\tau_{ext}^{aer,tr}(n) + \Delta\tau_{ext}^{mol}(n)} \\[2ex] \text{pcray}^{tr}(n) = \dfrac{\Delta\tau_{sca}^{mol}(n)}{\Delta\tau_{ext}^{aer,tr}(n) + \Delta\tau_{ext}^{mol}(n)} \end{cases}$$

4.3.4.2 Adjustment of the marine profile to the hydrosols phase function truncations

OSOAA calculates the marine profile (-**PROFILE_SEA.ResFile**) which provides for each level p:

- $\tau_{ext}(p)$: the extinction optical thickness
- pcwater(p): the mixing rate of water molecules for scattering
- pcsed(p): the mixing rate of mineral-like particles for scattering
- pcphyto(p): the mixing rate of phytoplankton for scattering

OSOAA calculates the radiative properties of mineral-like particles and phytoplankton particles (-**MLP.ResFile** and -**PHYTO.ResFile**) which include:s

- $\omega_0^{sed,tr}$: the mineral-like particles single scattering albedo adjusted to the mineral-like particles phase function truncation
- F^{sed} : the truncation coefficient for mineral-like particles
- $\omega_0^{phyto,tr}$: the phytoplankton single scattering albedo adjusted to the phytoplankton phase function truncation
- F^{phyto} : the truncation coefficient for phytoplankton particles

For a layer p, OSOAA calculates:

- The scattering optical thickness of mineral-like particles:

  Real value: $\Delta\tau_{sca}^{sed}(p) = \Delta\tau_{ext}(p) \times \text{pcsed}(p)$

  Value adjusted to the truncation: $\Delta\tau_{sca}^{sed,tr}(p) = \Delta\tau_{sca}^{sed}(p) \times (1 - F^{sed})$

- The scattering optical thickness of phytoplankton:

  Real value: $\Delta\tau_{sca}^{phyto}(p) = \Delta\tau_{ext}(p) \times \text{pcphyto}(p)$

  Value adjusted to the truncation: $\Delta\tau_{sca}^{phyto,tr}(p) = \Delta\tau_{sca}^{phyto}(p) \times (1 - F^{phyto})$

- The extinction optical thicknesses of mineral-like particles and phytoplankton adjusted to their phase function truncation:

$$\Delta\tau_{ext}^{sed,tr}(p) = \frac{\Delta\tau_{sca}^{sed,tr}(p)}{\omega_0^{sed,tr}} \qquad \Delta\tau_{ext}^{phyto,tr}(p) = \frac{\Delta\tau_{sca}^{phyto,tr}(p)}{\omega_0^{phyto,tr}}$$

- The scattering optical thickness of water molecules:

$$\Delta\tau_{sca}^{water}(p) = \Delta\tau_{ext}(p) \times \text{pcwater}(p)$$

- The absorption optical thickness of water molecules, yellow substance and detritus (only absorbing matters) :

$$\Delta\tau_{abs}^{mol+ys+det}(p) = \Delta\tau_{ext}(p) - \Delta\tau_{ext}^{sed}(p) - \Delta\tau_{ext}^{phyto}(p) - \Delta\tau_{sca}^{water}(p)$$

calculated from the real extinction optical thicknesses of mineral-like particles and phytoplankton (i.e. without phase function truncation adjustments):

$$\Delta\tau_{ext}^{sed}(p) = \frac{\Delta\tau_{ext}^{sed,tr}(p)}{1-\omega_0^{sed}\times F^{sed}} \qquad \Delta\tau_{ext}^{phyto}(p) = \frac{\Delta\tau_{ext}^{phyto,tr}(p)}{1-\omega_0^{phyto}\times F^{phyto}}$$

- The global extinction optical thickness adjusted to the truncations:

$$\tau_{ext}^{tr}(p) = \tau_{ext}^{tr}(p-1) + \Delta\tau_{ext}^{sed,tr}(p) + \Delta\tau_{ext}^{phyto,tr}(p) + \Delta\tau_{sca}^{water}(p) + \Delta\tau_{abs}^{mol+ys+det}(p)$$

- The scattering mixing rate adjusted to the truncations:

$$\begin{cases} pcsed^{tr}(p) = \dfrac{\Delta\tau_{sca}^{sed,tr}(p)}{\Delta\tau_{ext}^{sed,tr}(p)+\Delta\tau_{ext}^{phyto,tr}(p)+\Delta\tau_{sca}^{water}(p)+\Delta\tau_{abs}^{mol+ys+det}(p)} \\ pcphyto^{tr}(p) = \dfrac{\Delta\tau_{sca}^{phyto,tr}(p)}{\Delta\tau_{ext}^{sed,tr}(p)+\Delta\tau_{ext}^{phyto,tr}(p)+\Delta\tau_{sca}^{water}(p)+\Delta\tau_{abs}^{mol+ys+det}(p)} \\ pcwater^{tr}(p) = \dfrac{\Delta\tau_{sca}^{water}(p)}{\Delta\tau_{ext}^{sed,tr}(p)+\Delta\tau_{ext}^{phyto,tr}(p)+\Delta\tau_{sca}^{water}(p)+\Delta\tau_{abs}^{mol+ys+det}(p)} \end{cases}$$

4.4 Air / sea interface

This chapter presents the OSOAA modelling of the sea surface and its interactions with the polarized light coming from the atmospheric downwelling radiance field and from the marine upwelling one.

4.4.1 A complete modelling of polarized light interactions with the sea surface

OSOAA can simulate a flat sea surface as well as a rough sea surface.

Fresnel's laws are used to calculate the complete interactions of light with the sea surface:

- Reflection air → air — The reflection on the sea surface of the direct solar beam and diffuse light scattered in the atmosphere.
- Transmission air → sea — The transmission through the sea surface of the downwelling light coming from the atmosphere (direct solar light attenuated in the atmosphere and diffuse light scattered in the atmosphere).
- Reflection sea → sea — The reflection on the sea/surface interface, toward the sea bottom, of the upwelling light scattered in the water.
- Transmission sea → air — The transmission through the sea surface of the upwelling light coming from the sea water.

The direct solar beam, attenuated by the atmosphere and the diffuse light are both taken into account for a complete modelling of interactions with the sea surface.

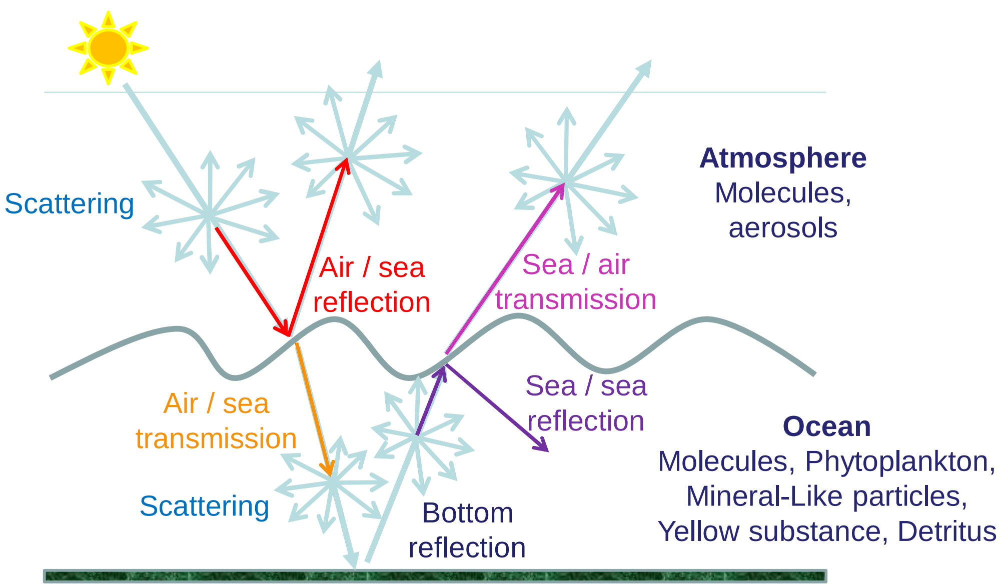


Figure 8 : Interactions of light on the sea surface interface, in the atmosphere and ocean, and on the bottom of the sea

4.4.2 Rough surface case

This chapter presents the mathematical formulation of the surface interaction matrices, introduced for a rough sea surface. OSOAA performs their expansion into Fourier series of the azimuth in order to use them on radiance fields expanded into same Fourier series.

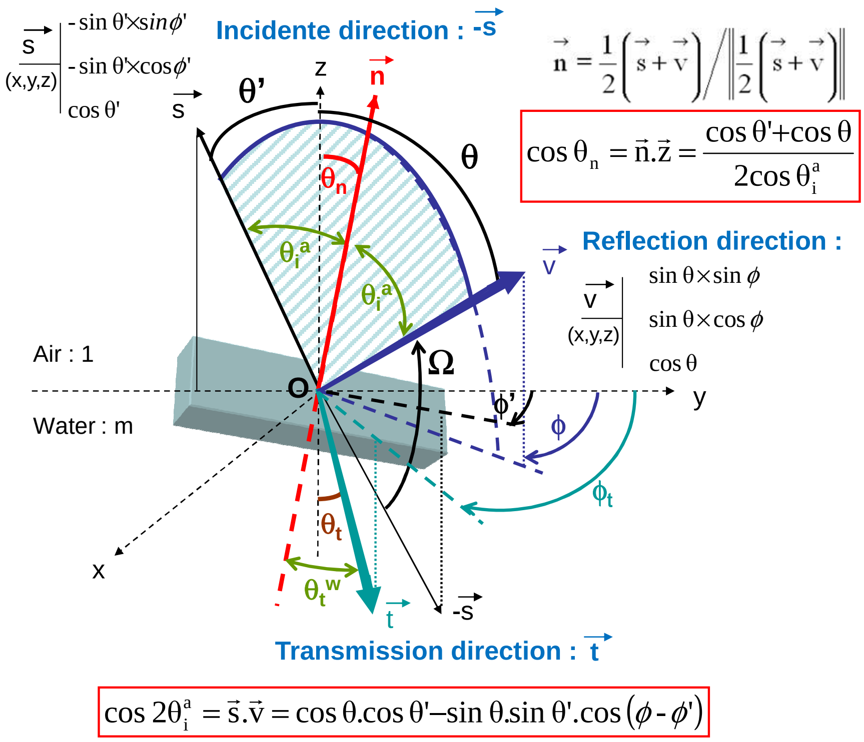
4.4.2.1 Modelling of the facets of waves

In case of a rough sea surface, waves are modelled according to the Cox and Munk probability for slopes of wind-driven waves [DR4]. The probability of an incident light beam in the direction (μ',ϕ') to meet a wave providing a reflexion toward the direction (μ,ϕ) is:

$$\boxed{p(\theta_n,\phi_n)=\frac{1}{\pi\sigma^2.\cos^3\theta_n}\times\exp\left(-\frac{\tan^2\theta_n}{\sigma^2}\right)} \qquad (54.a)$$

with $\sigma^2 = 0{,}003 + 0{,}00512 \times \text{wind (m/s)} \pm 0{,}004$ (54.b)

and θ_n the zenith angle of the direction $\vec{n}$ perpendicular to the facet of wave (see Figure 9)



θ_i^a : incidence angle (half angle between the incident and reflection directions).

θ_t^w : refractive angle (relative to the direction perpendicular to the facet of the wave).

θ_n : zenith angle of the direction perpendicular to the facet of wave on which occurs the reflexion from the incident direction to the reflection one.

θ_t : zenith angle of the transmission direction

Figure 9 : Rough sea surface interface - illustration of incident, reflection and transmission directions, in case of a downward incidence from the atmosphere (air→ sea)

4.4.2.2 Reflection air → air

The reflection of the direct solar beam and of the diffuse light on the sea surface, toward the direction (μ_r, ϕ_r), is given by:

$$\begin{cases} \text{Order 1: } \overline{\mathrm{L}}^{\uparrow}_{\mathrm{R1}}(\tau^*,\mu_r,\phi_r) = \dfrac{1}{4\pi.\mu_r} \times \overline{\overline{\mathrm{RAA}}}(\mu_r,\phi_r,\mu_0,\phi_0) \times \overline{E}.\exp(\tau^*/\mu_0) \\ \text{Order n: } \overline{\mathrm{L}}^{\uparrow}_{\mathrm{Rn}}(\tau^*,\mu_r,\phi_r) = \dfrac{1}{4\pi.\mu_r} \times \displaystyle\int_{\phi'=0}^{2\pi} \int_{\mu'=-1}^{0} \overline{\overline{\mathrm{RAA}}}(\mu_r,\phi_r,\mu',\phi') \times \overline{\mathrm{L}}^{\downarrow}_{\mathrm{n-1}}(\tau^*,\mu',\phi').d\mu'.d\phi' \end{cases} \tag{55}$$

with :

- $\mu' = -\cos\theta' < 0$ $(0 < \theta' < \pi/2)$: the cosine of the zenith angle of the downwelling incident light direction.
- ϕ' : the azimuth angle of the incident light direction.
- $\mu_0 < 0$: the cosine of the solar zenith angle.
- ϕ_0 : the azimuth angle of the solar incident direction.
- $\mu_r = \cos\theta > 0$ $(0 < \theta < \pi/2)$: the cosine of the zenith angle of the upwelling reflected light.
- ϕ_r : the azimuth angle of the reflected light direction.
- $\overline{\overline{\mathrm{RAA}}}(\mu_r,\phi_r,\mu',\phi')$ is the **air / air surface reflection matrix** for an incident beam toward the direction (μ', ϕ') and a reflection toward the direction (μ_r, ϕ_r).
- $\overline{\mathrm{L}}^{\uparrow}_{\mathrm{Rn}}(\tau^*,\mu,\phi) = \begin{pmatrix} \mathrm{I}^{\uparrow}_{\mathrm{Rn}}(\tau^*,\mu,\phi) \\ \mathrm{Q}^{\uparrow}_{\mathrm{Rn}}(\tau^*,\mu,\phi) \\ \mathrm{U}^{\uparrow}_{\mathrm{Rn}}(\tau^*,\mu,\phi) \end{pmatrix}$ is the Stokes vector of order n, resulting from the reflection on the sea surface (level 0+) of the incident light of order n-1.
- $\overline{E} = \begin{pmatrix} E \\ 0 \\ 0 \end{pmatrix}$ is the solar irradiance at TOA, toward the direction (μ_0, ϕ_0), which is attenuated from TOA to the sea surface by $\exp(\tau^*/\mu_0)$.

  Note : OSOAA calculates normalized radiance by using $E = \pi$.
- $\overline{\mathrm{L}}^{\downarrow}_{\mathrm{n-1}}(\tau^*,\mu',\phi')$ is the incident Stokes vector of order n-1 (diffuse incident light at the surface level).

The surface reflection follows the Fresnel's laws. Then, for a rough sea, the surface reflection matrix ***RAA*** includes the Fresnel reflection matrix ***RF_{AA}*** weighted by the probability function ***g*** of encoutering a facet of wave for the geometrical configuration of the incident and the reflection directions. Moreover, as we can easily express the Fresnel reflection matrix from a reference frame associated to the reflexion plane, the application of rotations is required to express the transition to frames associated to the incident meridian plane and to the reflection meridian plane from the reflexion plane :

$$\boxed{\overline{\overline{\mathrm{RAA}}}(\mu_r,\phi_r,\mu',\phi') = \mathrm{g_R}(\mu_r,\phi_r,\mu',\phi') \times \overline{\overline{\Re}}(-\chi).\overline{\overline{\mathrm{RF}}}_{\mathrm{AA}}(i^a).\overline{\overline{\Re}}(\chi').} \quad (56)$$

with :

- $$\boxed{g_R(\mu_r,\phi_r,\mu',\phi') = \frac{1}{\sigma^2.\cos^4\theta_n} \times \exp\left(-\frac{\tan^2\theta_n}{\sigma^2}\right)} \quad (57)$$

  where : σ^2 =0,003 + 0,00512 × wind (m/s)

- χ' : the rotation angle between the direction perpendicular to the incident meridian plane and the direction perpendicular to the reflection plane.

- $-\chi$: the rotation angle between the direction perpendicular to the reflection plane and the direction perpendicular to the reflection meridian plane.

- $\overline{\overline{\Re}}(\chi')$ the rotation matrix: $$\boxed{\overline{\overline{\Re}}(\chi') = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos 2\chi' & \sin 2\chi' \\ 0 & -\sin 2\chi' & \cos 2\chi' \end{pmatrix}} \quad (58)$$

- $\overline{\overline{\mathrm{RF}}}_{\mathrm{AA}}(i^a)$ is the Fresnel reflection matrix (air → air reflection) for a reference frame associated to the reflection plane, with i^a the incidence angle from the atmosphere relative to the vector perpendicular to the facet of the wave:

$$\boxed{\overline{\overline{\mathrm{RF}}}_{\mathrm{AA}}(\cos i^a) = \left(\begin{array}{c|c|c} \mathrm{R}_{11}^{\mathrm{th}}(i^a) & \mathrm{R}_{12}^{\mathrm{th}}(i^a) & 0 \\ \hline \mathrm{R}_{12}^{\mathrm{th}}(i^a) & \mathrm{R}_{11}^{\mathrm{th}}(i^a) & 0 \\ \hline 0 & 0 & \mathrm{R}_{33}^{\mathrm{th}}(i^a) \end{array}\right)} \quad (59.a)$$

with

$$\boxed{\begin{aligned} \mathrm{R}_{11}^{\mathrm{th}}(i^a) &= 0.5\times\left[\left(\mathrm{r}_\ell^{\mathrm{th}}(i^a)\right)^2 + \left(\mathrm{r}_\mathrm{r}^{\mathrm{th}}(i^a)\right)^2\right] \\ \mathrm{R}_{12}^{\mathrm{th}}(i^a) &= 0.5\times\left[\left(\mathrm{r}_\ell^{\mathrm{th}}(i^a)\right)^2 - \left(\mathrm{r}_\mathrm{r}^{\mathrm{th}}(i^a)\right)^2\right] \\ \mathrm{R}_{33}^{\mathrm{th}}(i^a) &= \mathrm{r}_\ell^{\mathrm{th}}(i^a)\times\mathrm{r}_\mathrm{r}^{\mathrm{th}}(i^a) \end{aligned}} \quad (59.b)$$

where $$\boxed{r_\ell^{th}(i^a) = \frac{m^2.\cos i^a - \sqrt{m^2 - \sin^2(i^a)}}{m^2.\cos i^a + \sqrt{m^2 - \sin^2(i^a)}}} \quad (59.c)$$

$$\boxed{r_r^{th}(i^a) = \frac{\cos i^a - \sqrt{m^2 - \sin^2(i^a)}}{\cos i^a + \sqrt{m^2 - \sin^2(i^a)}}} \quad (59.d)$$

The incident angle i^a, relative to the direction perpendicular to the facet of the wave, is given by (cf. Figure 9, p 100) :

$$\boxed{\cos 2\,i^a = \cos\theta.\cos\theta' - \sin\theta.\sin\theta'.\cos(\phi - \phi')} \quad (60)$$

4.4.2.3 Transmission air → sea

Similary to the reflexion, the transmission through the sea surface of the direct solar beam and of the diffuse light on the sea surface, toward the direction (μ_t, ϕ_t), is given by :

$$\begin{cases} \text{Order 1: } \overline{L}_{T1}^{\downarrow 0-}(\tau^*, \mu_t, \phi_t) = \dfrac{1}{\pi.\mu_t} \times \overline{\overline{TAW}}(\mu_t, \phi_t, \mu_0, \phi_0).\overline{E}.\exp(\tau^* / \mu_0) \\ \text{Order n: } \overline{L}_{Tn}^{\downarrow 0-}(\tau^*, \mu_t, \phi_t) = \dfrac{1}{\pi.\mu_t} \times \int_0^{2\pi}\int_{-1}^{0} \overline{\overline{TAW}}(\mu_t, \phi_t, \mu', \phi').\overline{L}_{n-1}^{\downarrow 0+}(\tau^*, \mu', \phi').d\mu'.d\phi' \end{cases}$$

(61)

with :

- $\mu_t = \cos\theta_t < 0$ ($0 < \theta_t < \pi/2$): the cosine of the zenith angle of the downwelling transmitted light.
- ϕ_t : the azimuth angle of the transmitted light.
- $\overline{\overline{TAW}}(\mu_t, \phi_t, \mu', \phi')$ is the **air / sea transmission matrix** for an incident beam toward the direction (μ', ϕ') and a transmission toward the direction (μ_t, ϕ_t)..
- $\overline{L}_{Tn}^{\downarrow 0-}(\tau^*, \mu_t, \phi_t)$ is the Stokes vector of order n, just below the sea surface (called level 0-), resulting from the transmission through the surface of the incident light of order n-1.

The air → sea water transmission matrix **TAW** is given by:

$$\boxed{\overline{\overline{TAW}}(\mu_t, \phi_t, \mu', \phi') = g_T(\mu_t, \phi_t, \mu', \phi') \times \overline{\overline{\Re}}(-\chi_t).\overline{\overline{TF}}_{AW}^{FLUX}(i^a).\overline{\overline{\Re}}(\chi_t') \times \frac{m^2.\cos t^w.\cos i^a}{(m.\cos t^w - \cos i^a)^2}}$$

(62)

with :

- i^a : the incidence angle from the atmosphere relative to the vector perpendicular to the facet of the wave.

- t^w : the refraction angle into the sea relative to the vector perpendicular to the facet of the wave.

$$\boxed{\sin i^a = m.\sin t^w} \qquad (63)$$

- χ_t' : the rotation angle between the direction perpendicular to the incident meridian plane and the direction perpendicular to the transmission plane.

- $-\chi_t$: the rotation angle between the direction perpendicular to the transmission plane and the direction perpendicular to the transmission meridian plane.

- gt(μ_t, ϕ_t, μ', ϕ') : the probability function of encountering a facet of wave for the incident direction (μ', ϕ') and the transmission direction (μ_t, ϕ_t). As a given incident direction on a given oriented facet of wave occurs a single configuration of reflection direction and transmission direction, there is the following relation:

$$\boxed{g_T(\mu_t, \phi_t, \mu', \phi') = g_R(\mu_r, \phi_r, \mu', \phi')} \qquad (64)$$

- $\overline{\overline{\mathrm{TF}}}_{\mathrm{AW}}^{\mathrm{FLUX}}\left(\cos i^a\right)$ is the Fresnel transmission matrix (air $\rightarrow$ sea transmission) for a reference frame associated to the transmission plane:

$$\boxed{\overline{\overline{\mathrm{TF}}}_{\mathrm{AW}}^{\mathrm{FLUX}}\left(\cos i^a\right) = \frac{\mathrm{m}.\cos t^w}{\cos i^a} \times \begin{pmatrix} t_{11}^{th}(i^a) & t_{12}^{th}(i^a) & 0 \\ t_{12}^{th}(i^a) & t_{11}^{th}(i^a) & 0 \\ 0 & 0 & t_{33}^{th}(i^a) \end{pmatrix}} \qquad (65.a)$$

with

$$\boxed{\begin{aligned} t_{11}^{th}(i^a) &= 0.5 \times \left[\left(t_\ell^{th}(i^a)\right)^2 + \left(t_r^{th}(i^a)\right)^2\right] \\ t_{12}^{th}(i^a) &= 0.5 \times \left[\left(t_\ell^{th}(i^a)\right)^2 - \left(t_r^{th}(i^a)\right)^2\right] \\ t_{33}^{th}(i^a) &= t_\ell^{th}(i^a) \times t_r^{th}(i^a) \end{aligned}} \qquad (65.b)$$

where

$$\boxed{t_\ell^{th}(i^a) = \frac{1}{\mathrm{m}} \times \left(1 + r_\ell^{th}(i^a)\right)} \qquad (65.c)$$

$$\boxed{t_r^{th}(i^a) = 1 + r_r^{th}(i^a)} \qquad (65.d)$$

For a couple of incident direction (μ', ϕ') and the transmission direction (μ_t, ϕ_t) the Fresnel incidence angle i^a is calculated from geometrical considerations.

4.4.2.4 Reflection sea → sea

The upwelling sea radiance is only a diffuse light. Indeed, the direct solar beam is a downward illumination which is scattered in the sea water or reflected by the bottom of the sea (assumed to be a lambertian surface).

The reflection under the surface of the upwelling sea light, toward the direction (μ_r, ϕ_r), is given by:

$$\boxed{\begin{aligned}&\overline{\mathrm{L}}^{\downarrow sea}_{\mathrm{R}\,n}(0\text{-},\mu_r,\phi_r)\\&=\frac{1}{4\pi.(-\mu_r)}\times\int_{\phi'=0}^{2\pi}\int_{\mu'=0}^{1}\overline{\overline{\mathrm{RWW}}}(\mu_r,\phi_r,\mu',\phi').\overline{\mathrm{L}}^{\uparrow sea}_{n-1}(0\text{-},\mu',\phi').d\mu'.d\phi'\end{aligned}} \quad (66)$$

with :

- $\mu'>0$: the cosine of the zenith angle of the upwelling incident light direction.
- ϕ' : the azimuth angle of the incident light direction.
- $\mu_r < 0$: the cosine of the zenith angle of the downwelling reflected light.
- ϕ_r : the azimuth angle of the reflected light.
- $\overline{\overline{\mathrm{RWW}}}(\mu_r,\phi_r,\mu',\phi')$ is the **sea / sea surface reflection matrix** for an incident beam toward the direction (μ', ϕ') and a reflection toward the direction (μ_r, ϕ_r).
- $\overline{\mathrm{L}}^{\downarrow sea}_{\mathrm{R}\,n}(0\text{-},\mu,\phi)$ is the Stokes vector of order n, resulting from the reflection on the sea surface (level 0-) of the upwelling incident light of order n-1.
- $\overline{\mathrm{L}}^{\uparrow sea}_{n-1}(0\text{-},\mu',\phi')$ is the incident Stokes vector of order n-1 (diffuse upwelling light at sea surface : level 0-).

The surface reflection sea → sea ***RWW*** is calculated from the Fresnel reflection matrix ***RF***$_{WW}$ weighted by the probability function ***g*** of slope waves and by taking into account for rotations to bring the frame associated to the incident meridian plane to the frame associated to the reflection meridian plane, via the reflection plane.

$$\boxed{\overline{\overline{\mathrm{RWW}}}(\mu,\phi,\mu',\phi')=g_R(\mu_r,\phi_r,\mu',\phi')\times\overline{\overline{\Re}}(-\chi_w).\overline{\overline{\mathrm{RF}}}_{\mathrm{WW}}(i^w).\overline{\overline{\Re}}(\chi_w')} \quad (67)$$

with :

- $\boxed{g_R(\mu_r,\phi_r,\mu',\phi')=\frac{1}{\sigma^2.\cos^4\theta_n}\times\exp\left(-\frac{\tan^2\theta_n}{\sigma^2}\right)}$ defines by the same equation as (57), but for zenith angles of the direction perpendicular to the facets of waves which are calculated for $\mu'>0$ and $\mu_r<0$

- χ_w' : the rotation angle between the direction perpendicular to the incident meridian plane and the direction perpendicular to the reflection plane.
- $-\chi_w$: the rotation angle between the direction perpendicular to the reflection plane and the direction perpendicular to the reflection meridian plane.
- $\overline{\overline{\Re}}(\chi')$ the rotation matrix defined by equation (58).
- $\overline{\overline{\mathrm{RF}}}\mathrm{ww}(i^w)$ is the Fresnel reflection matrix (sea → sea reflection) for a reference frame associated to the reflection plane, with i^w the incidence angle from the sea water relative to the vector perpendicular to the facet of the wave:

$$\overline{\overline{\mathrm{RF}}}\mathrm{ww}(\cos i^w) = \begin{pmatrix} \mathrm{R}_{11}^{\mathrm{th}}(i^w) & \mathrm{R}_{12}^{\mathrm{th}}(i^w) & 0 \\ \mathrm{R}_{12}^{\mathrm{th}}(i^w) & \mathrm{R}_{11}^{\mathrm{th}}(i^w) & 0 \\ 0 & 0 & \mathrm{R}_{33}^{\mathrm{th}}(i^w) \end{pmatrix} \qquad (68.a)$$

with

$$\begin{aligned} \mathrm{R}_{11}^{\mathrm{th}}(i^w) &= 0.5 \times \left[\left(\mathrm{r}_\ell^{\mathrm{th}}(i^w)\right)^2 + \left(\mathrm{r}_\mathrm{r}^{\mathrm{th}}(i^w)\right)^2 \right] \\ \mathrm{R}_{12}^{\mathrm{th}}(i^w) &= 0.5 \times \left[\left(\mathrm{r}_\ell^{\mathrm{th}}(i^w)\right)^2 - \left(\mathrm{r}_\mathrm{r}^{\mathrm{th}}(i^w)\right)^2 \right] \\ \mathrm{R}_{33}^{\mathrm{th}}(i^w) &= \mathrm{r}_\ell^{\mathrm{th}}(i^w) \times \mathrm{r}_\mathrm{r}^{\mathrm{th}}(i^w) \end{aligned} \qquad (68.b)$$

where

$$\mathrm{r}_\ell^{\mathrm{th}}(i^w) = \frac{\cos i^w - \mathrm{m} \times \sqrt{1 - \mathrm{m}^2 . \sin^2\left(i^w\right)}}{\cos i^w + \mathrm{m} \times \sqrt{1 - \mathrm{m}^2 . \sin^2\left(i^w\right)}} \qquad (68.c)$$

$$\mathrm{r}_r^{\mathrm{th}}(i^w) = \frac{\mathrm{m}.\cos i^w - \sqrt{1 - \mathrm{m}^2 . \sin^2\left(i^w\right)}}{\mathrm{m}.\cos i^w + \sqrt{1 - \mathrm{m}^2 . \sin^2\left(i^w\right)}} \qquad (68.d)$$

Note : Case of a total reflection

For an incidence angle i^w greater than the limit angle, defined by $m.\sin i_{\mathrm{lim}}^w = 1$, there is a total reflexion:

$$\begin{cases} \mathrm{R}_{11}^{\mathrm{th}}(i^w > i_{\mathrm{lim}}^w) = 1 \\ \mathrm{R}_{12}^{\mathrm{th}}(i^w > i_{\mathrm{lim}}^w) = 0 \\ \mathrm{R}_{33}^{\mathrm{th}}(i^w > i_{\mathrm{lim}}^w) = 1 \end{cases} \qquad (68.e)$$

The incident angle i^w relative to the direction perpendicular to the facet of the wave is given by (cf. Figure 10):

$$\boxed{\cos 2\, i^w = \cos\theta.\cos\theta' - \sin\theta.\sin\theta'.\cos(\phi - \phi')} \qquad (69)$$

The **incidence direction** is given by the vector $-\vec{s}$ with:

- a zenith angle θ' defined between 0 and π/2
- an azimuth angle ϕ'

The **transmission direction** is given by the vector $\vec{t}$ with:

- a zenith angle θ_t defined between 0 and π/2
- an azimuth angle ϕ_t

The **reflexion direction** is given by the vector $\vec{v}$ with:

- a zenith angle θ defined between 0 and π/2
- an azimuth angle ϕ

The **direction perpendicular** to the facet of the **wave** is given by the vector $\vec{n}$ with:

- a zenith angle θ_n defined between 0 and π/2
- an azimuth angle ϕ_n

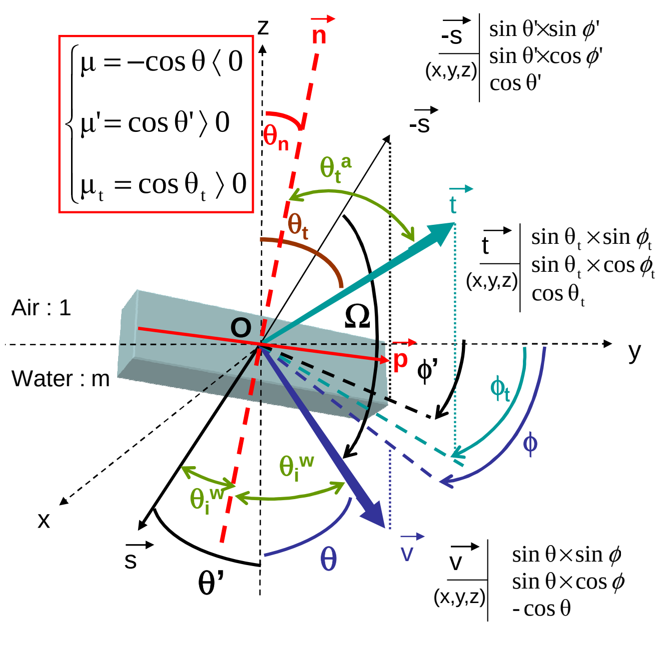


Figure 10 : illustration of incident, reflection and transmission directions, in case of an upward incidence from the sea (sea → air transition for a rough sea surface)

4.4.2.5 Transmission sea → air

The transmission through the sea surface of upwelling sea radiance, toward the direction (μ_t, ϕ_t), is given by:

$$\boxed{\begin{aligned}&\overline{L}^{\uparrow sea}_{Tn}(0+,\mu_t,\phi_t)\\ &= \frac{1}{\pi.\mu_t} \times \int_{\phi'=0}^{2\pi} \int_{\mu'=0}^{1} \overline{\overline{TWA}}(\mu_t,\phi_t,\mu',\phi').\overline{L}^{\uparrow sea}_{n-1}(0-,\mu',\phi').d\mu'.d\phi'\end{aligned}} \qquad (70)$$

with :

- $\mu_t = \cos\theta_t < 0$ ($0 < \theta_t < \pi/2$): the cosine of the zenith angle of the upwelling transmitted light.
- ϕ_t : the azimuth angle of the transmitted light direction.
- $\overline{\overline{\mathrm{TWA}}}(\mu_t, \phi_t, \mu', \phi')$ is the **sea / air transmission matrix** for an incident beam toward the direction (μ', ϕ') and a transmission toward the direction (μ_t, ϕ_t)..
- $\overline{\mathrm{L}}_{\mathrm{Tn}}^{\uparrow sea}(0+, \mu_t, \phi_t)$ is the Stokes vector of order n, just above the sea surface (level 0+), resulting from the transmission through the surface of the incident light of order n-1.

The sea → air transmission matrix **TWA** is given by:

$$\boxed{\overline{\overline{\mathrm{TWA}}}(\mu_t, \phi_t, \mu', \phi') = g_T(\mu_t, \phi_t, \mu', \phi') \times \frac{\cos t^a . \cos i^w}{(m.\cos i^w - \cos t^a)^2} \times \overline{\overline{\Re}}(-\chi_{wt}) . \overline{\overline{\mathrm{TF}}}_{\mathrm{WA}}^{\mathrm{FLUX}}(i^w) . \overline{\overline{\Re}}(\chi_{wt}')} \tag{71}$$

with :

- i^w : the incidence angle from the sea relative to the vector perpendicular to the facet of the wave.
- t^a : the refraction angle into the air relative to the vector perpendicular to the facet of the wave.
- χ_{wt}' : the rotation angle between the direction perpendicular to the incident meridian plane and the direction perpendicular to the transmission plane.
- $-\chi_{wt}$: the rotation angle between the direction perpendicular to the transmission plane and the direction perpendicular to the transmission meridian plane.
- $g_T(\mu_t, \phi_t, \mu', \phi')$: the probability function of encountering a facet of wave for the incident direction (μ', ϕ') and the transmission direction (μ_t, ϕ_t). We notice:

$$\boxed{g_T(\mu_t, \phi_t, \mu', \phi') = g_R(\mu_r, \phi_r, \mu', \phi')} \tag{72}$$

- $\overline{\overline{\mathrm{TF}}}_{\mathrm{WA}}^{\mathrm{FLUX}}(i^w)$ is the Fresnel transmission matrix (sea → air transmission) for a reference frame associated to the transmission plane:

$$\boxed{\overline{\overline{\mathrm{TF}}}_{\mathrm{WA}}^{\mathrm{FLUX}}(\cos i^w) = \frac{\cos t^a}{\mathrm{m}.\cos i^w} \times \begin{pmatrix} t_{11}^{th}(i^w) & t_{12}^{th}(i^w) & 0 \\ t_{12}^{th}(i^w) & t_{11}^{th}(i^w) & 0 \\ 0 & 0 & t_{33}^{th}(i^w) \end{pmatrix}} \tag{73.a}$$

with

$$\boxed{\begin{aligned} t_{11}^{th}(i^w) &= 0.5\times\left[\left(t_\ell^{th}(i^w)\right)^2+\left(t_r^{th}(i^w)\right)^2\right] \\ t_{12}^{th}(i^w) &= 0.5\times\left[\left(t_\ell^{th}(i^w)\right)^2-\left(t_r^{th}(i^w)\right)^2\right] \\ t_{33}^{th}(i^w) &= t_\ell^{th}(i^w)\times t_r^{th}(i^w) \end{aligned}} \quad (73.b)$$

where $\boxed{t_\ell^{th}(i^w) = m\times\left(1+r_\ell^{th}(i^w)\right)}$ (73.c) $\boxed{t_r^{th}(i^w) = 1+r_r^{th}(i^w)}$ (73.d)

The Fresnel incidence angle i^w is calculated from geometrical considerations.

Note : Case of a total reflection

There is a transmission from the sea water to the air only if $m.\sin i^w \leq 1$.

In this case, the refraction angle t^a into the air relative to the vector perpendicular to the facet of the wave is:

$$\boxed{\sin t^a = m.\sin i^w} \quad (74)$$

In the opposite case, there is a total reflexion and no transmission.

5. Validation of the OSOAA model

The validation of profiles, radiative properties of aerosols or hydrosols, and successive orders of scattering calculations have been first performed by comparing OSOAA simulations for a flat sea to the original OSOA code (only available for a flat sea condition) which has been validated elsewhere [Chami et al., 2001]. A very good agreement has been obtained. It is not discussed here since this chapter focuses on the validation of the new implementation of the rough sea surface within the model OSOAA.

5.1 Validation of the full reflexion/transmission Mueller matrix for a rough sea surface

This validation stands on an inter comparison of simulations with the model of Jacek Chowdhary [DR3], hereafter noted as JC's code. Global radiance fields, for Stokes parameters (I,Q,U), are compared in order to validate the correct implementation of the diffuse and solar direct light reflexion/transmission through the air/sea interface. These simulations take into account all scattering processes as well as all the air / sea and sea / air interactions for a rough sea surface. OSOAA and JC's code simulations of Stokes vector (I,Q,U) are compared at the **sea surface level 0+** and at **TOA** for upwelling directions.

5.1.1 Conditions of the simulations

The conditions of the simulations are as follows:

- Solar zenith angle: 30° and 60°
- Spectral bands: 412 nm and 660 nm
- Gauss angles:

  Table 13 shows the values of the cosine of Gauss angles and their weight for spatial integrations. 40 Gauss angles are used and three specific angles are added with a null weight: the nadir direction, the solar zenith angle in the air and in the sea.
- Atmospheric scattering by molecules (no aerosols).

  Table 14 shows the values of the atmospheric Rayleigh optical versus the wavelength.
- Oceanic components: only water molecules (i.e. no particle or CDOM)

  Table 14 shows the values of the absorption and scattering coefficients (a_w and b_w) for a pure sea water versus the wavelength.
- The factor of molecular depolarization in the air and in the sea is null.
- Sea depth: 1000 m.
- Wind velocity at surface level: 7 m/s
- Sea bottom albedo: 0.
- Wave distribution of Cox and Munk model
- No shadowing effect of waves (functionality cut off for JC's code)
- No foam

Table 13 : Cosine of used Gauss angles and associated weights. Three specific angles are added with a null weight: nadir direction, solar zenith angle in the air (here 60°) and in the sea

Ind	Cosine of the angle	Weight
1	0.10000000000000E+01	0.00000000000000E+00
2	0.99955382265163E+00	0.11449500031887E-02
3	0.99764986439824E+00	0.26635335895143E-02
4	0.99422754096569E+00	0.41803131246912E-02
5	0.98929130249976E+00	0.56909224514043E-02
6	0.98284857273863E+00	0.71929047681184E-02
7	0.97490914058573E+00	0.86839452692619E-02
8	0.96548508904380E+00	0.10161766041103E-01
9	0.95459076634363E+00	0.11624114120797E-01
10	0.94224276130987E+00	0.13068761592400E-01
11	0.92845987717245E+00	0.14493508040509E-01
12	0.91326310257176E+00	0.15896183583725E-01
13	0.89667557943877E+00	0.17274652056270E-01
14	0.87872256767821E+00	0.18626814208300E-01
15	0.85943140666311E+00	0.19950610878142E-01
16	0.83883147358026E+00	0.21244026115782E-01
17	0.81695413868146E+00	0.22505090246332E-01
18	0.79383271750461E+00	0.23731882865930E-01
19	0.76950242013504E+00	0.24922535764116E-01
20	0.76309391230831E+00	0.00000000000000E+00
21	0.74400029758360E+00	0.26075235767565E-01
22	0.71736518536210E+00	0.27188227500486E-01
23	0.68963764434203E+00	0.28259816057277E-01
24	0.66085989898612E+00	0.29288369583267E-01
25	0.63107577304687E+00	0.30272321759558E-01
26	0.60033062282975E+00	0.31210174188115E-01
27	0.56867126812271E+00	0.32100498673488E-01
28	0.53614592089713E+00	0.32941939397646E-01
29	0.50280411188878E+00	0.33733214984612E-01
30	0.50000000000000E+00	0.00000000000000E+00
31	0.46869661517054E+00	0.34473120451754E-01
32	0.43387537083176E+00	0.35160529044748E-01
33	0.39839340588197E+00	0.35794393953416E-01
34	0.36230475349949E+00	0.36373749905836E-01
35	0.32566437074770E+00	0.36897714638276E-01
36	0.28852805488451E+00	0.37365490238731E-01
37	0.25095235839227E+00	0.37776364362001E-01
38	0.21299450285767E+00	0.38129711314478E-01
39	0.17471229183265E+00	0.38424993006959E-01
40	0.13616402280914E+00	0.38661759774076E-01
41	0.97408398441585E-01	0.38839651059052E-01
42	0.58504437152421E-01	0.38958395962770E-01
43	0.19511383256794E-01	0.39017813656307E-01

Table 14 : Molecular optical thickness of the atmosphere ($\tau_{Rayleigh}$), absorption coefficient (a_w) and scattering one (b_w) for a pure sea water, for the different wavelengths of simulation

	412 nm	443 nm	490 nm	550 nm	660 nm
$\tau_{Rayleigh}$	0.314125824	0.232630014	0.153598466	0.0957390344	0.045615378
a_w (m^{-1})	0.00455056	0.00706914	0.015	0.0565	0.41
b_w (m^{-1})	0.00665	0.00487235	0.00316451	0.00193224	0.000889028

5.1.2 Results

Output results are compared at the sea surface level 0+ and at TOA, in the half-planes of azimuth: 0° and 180° (solar principal plane) and 90° (perpendicular to the solar principal plane).

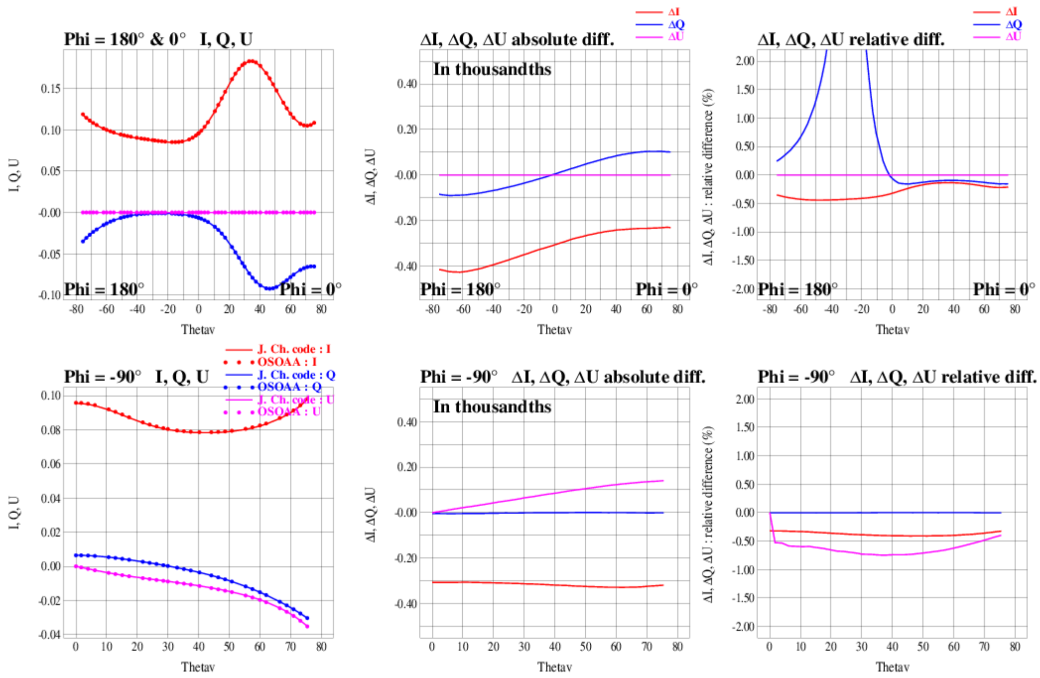
For upward radiance just above the sea surface (level 0+):

- At 412 nm, the molecular scattering is the strongest; therefore sea surface interactions with the diffuse light are important. Figure 11 shows the Stokes parameters (I,Q,U) simulated by OSOAA are very close to those simulated by the JC's code: absolute differences are lower than 0.4×10^{-3} of normalized radiance for the intensity I and lower than 0.1×10^{-3} for parameters Q and U. The relative differences do not exceed 0.8%, except for the parameters Q and U within directions for which the polarization trends to be null (in this latter case, the relative difference is meaningless).
- Figure 12 shows that at 660 nm, for weaker scattering effects, the absolute differences do not exceed 0.02×10^{-3} of normalized radiance.

For upwelling radiance at TOA:

- At 443 nm (Figure 13), absolute differences at TOA are similar to those obtained at level 0+, which leads to lower relative differences reaching at most 0.2% for I, because the upwelling TOA signal is higher than the surface one (mainly for the intensity). Same results are obtained for Q and U, again except within the range of directions for which Q or U is close to be null.
- At 660 nm, absolute differences at TOA only reaches up to 0.05 to 0.1×10^{-3} of normalized radiance for the intensity I and slightly less for Q and U parameters.

Simulation case : 3 SZA : 30 Wavelength : 412 SRF W07



Simulation case : 3 SZA : 60 Wavelength : 412 SRF W07

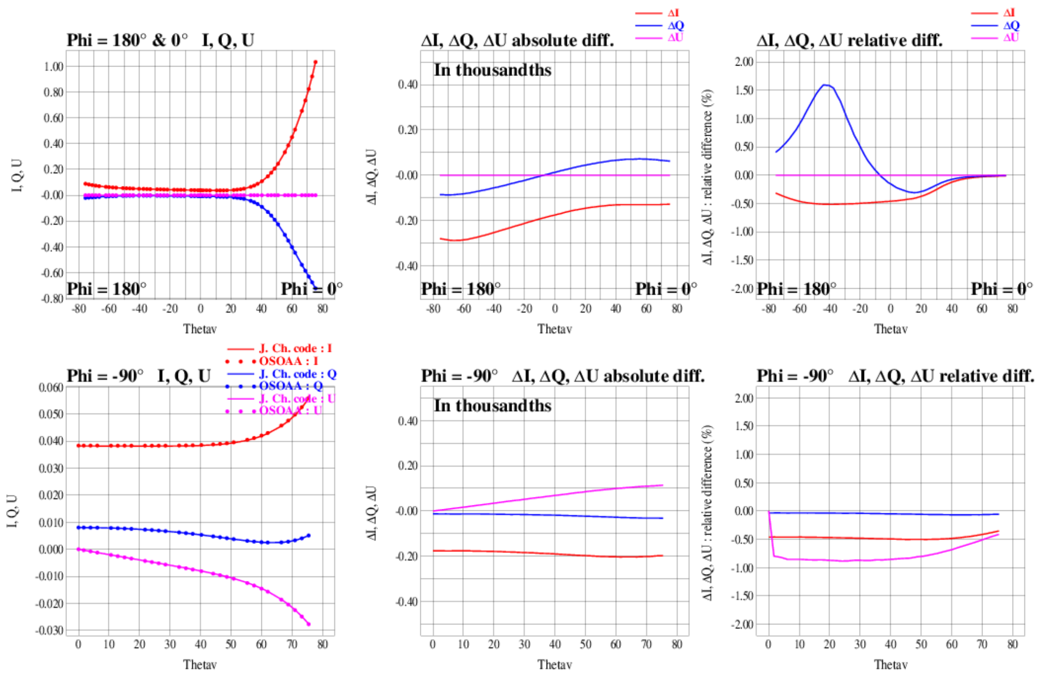
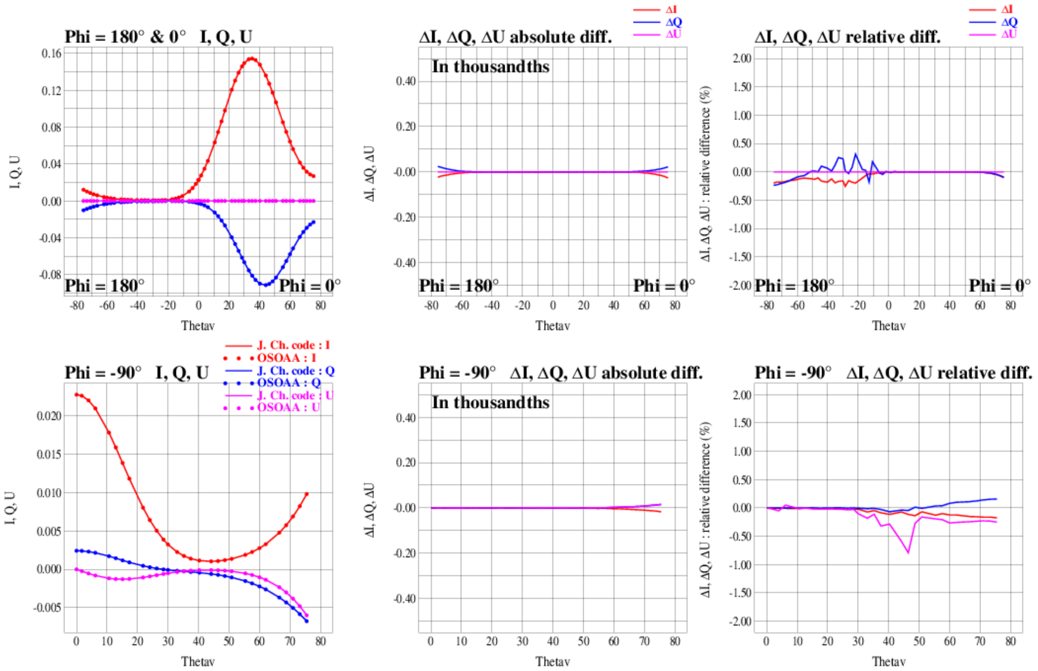


Figure 11 : Upward normalized radiance (I,Q,U) at 412-nm, at sea surface level 0+, simulated by OSOAA and by the JC's code (left column), absolute difference (middle column) and relative difference (right column). The first line shows results in the solar principal plan. The second one shows results in the perpendicular plane. Simulations for a SZA =30° and 60°.

Simulation case : 3 SZA : 30 Wavelength : 660 SRF W07



Simulation case : 3 SZA : 60 Wavelength : 660 SRF W07

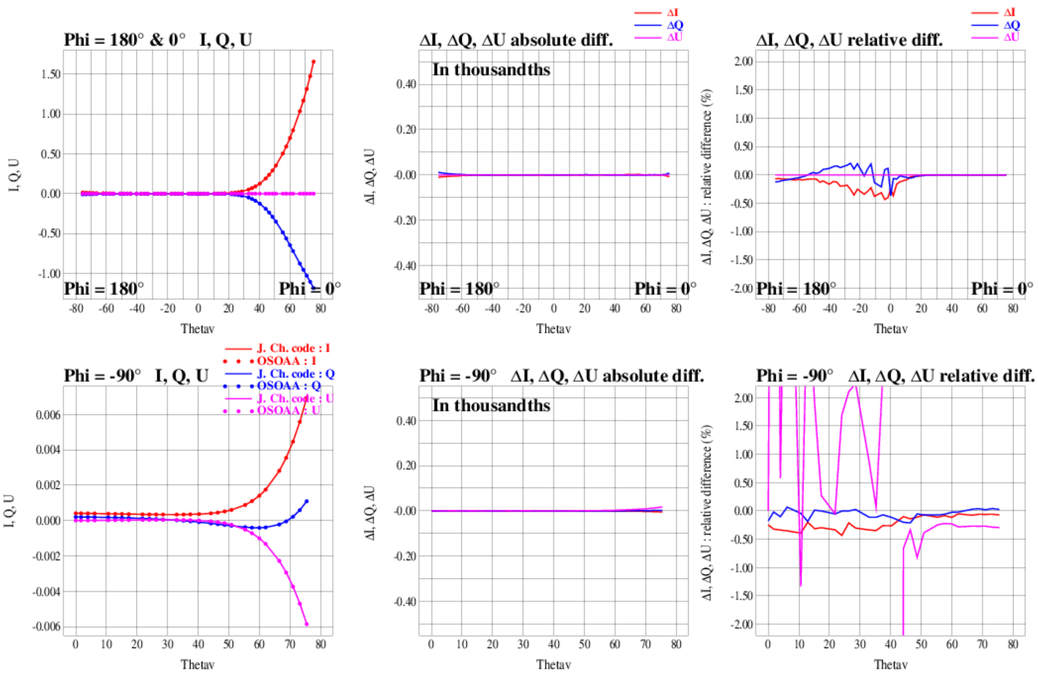


Figure 12 : Same legend as Figure 11 but at 670-nm.

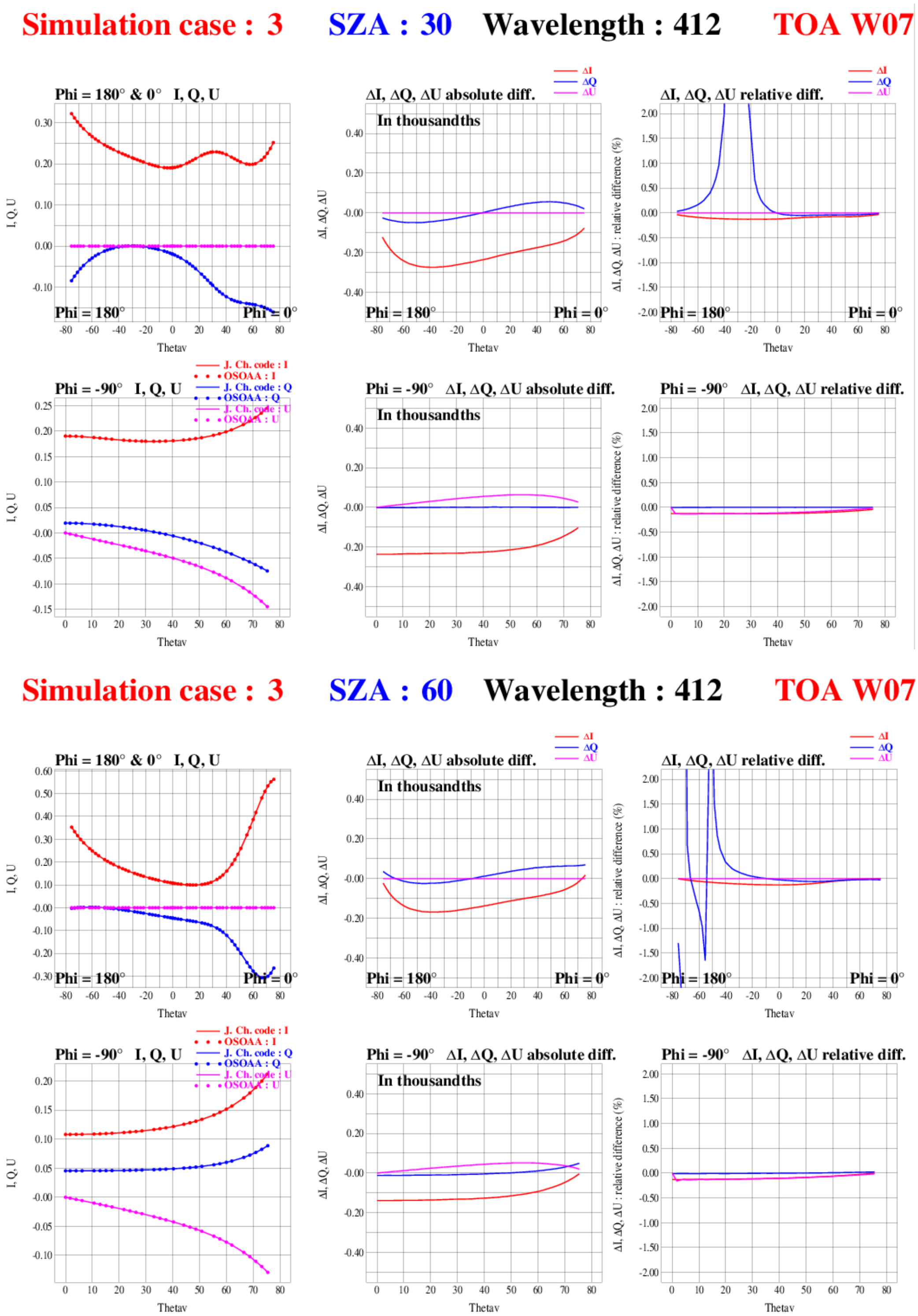
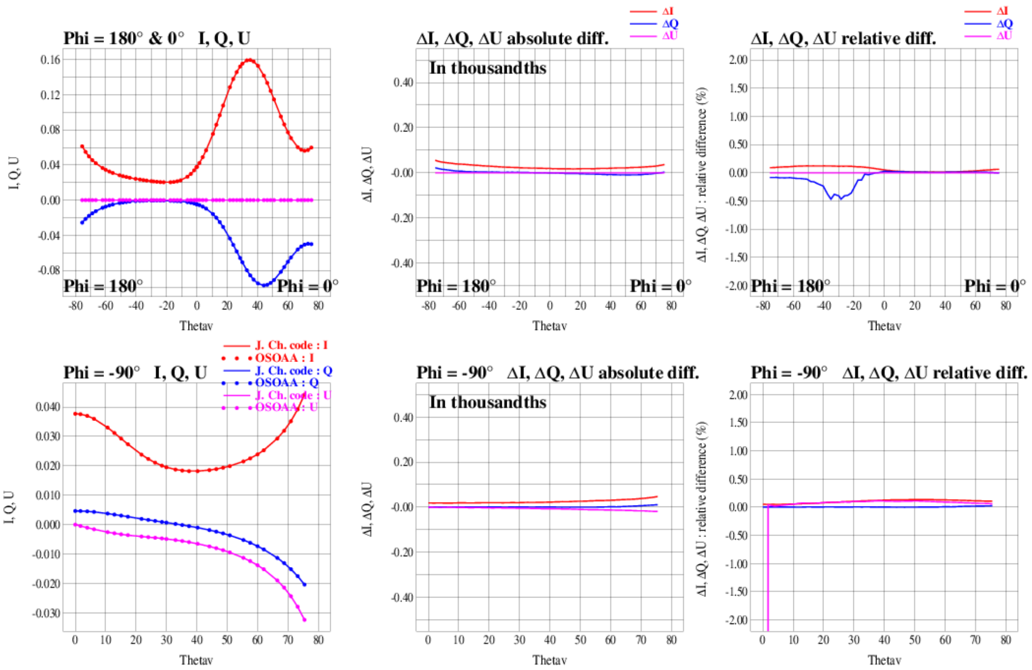


Figure 13 : Same legend as Figure 11 but simulation at TOA level.

Simulation case : 3 SZA : 30 Wavelength : 660 TOA W07



Simulation case : 3 SZA : 60 Wavelength : 660 TOA W07

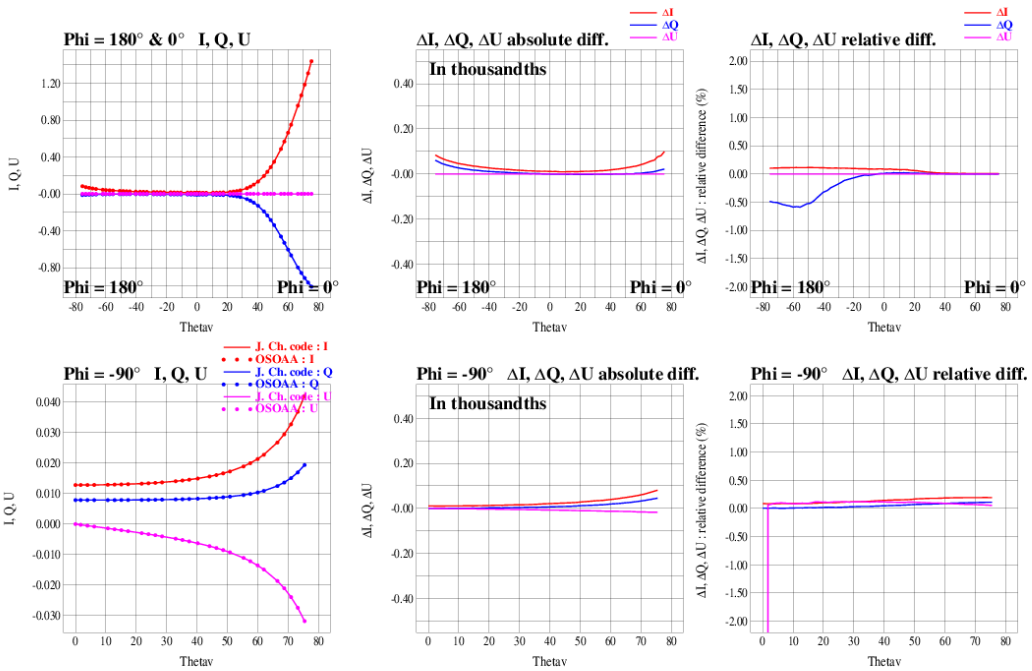


Figure 14 : Same legend as Figure 11 but at TOA level and at 670-nm.

5.2 Validation of the conservation of energy through the reflexion/transmission Mueller matrix

This validation aims at checking the conservation of energy within OSOAA model when light is reflected and transmitted through the sea surface, in the case of a rough sea.

Indeed, the conservation budget of radiance fluxes at the air/sea interface is a good test to exhibit the consistency of the radiative transfert code. A validation test is then performed by comparing the incident, reflected and transmitted fluxes at the interface, for conservative atmosphere and marine environments (i.e. non absorbing environments).

The incident flux on the sea surface (level 0+), noted $F_{total}^{0+,down}$, is the combination of the direct solar irradiance, attenuated by its propagation throught the atmosphere, and the downwelling diffuse light scattered in the atmosphere. The upwelling flux at level 0+, $F_{total}^{0+,up}$, corresponds to the reflection of the atmospheric light and to the transmission of the marine diffuse ligtht through sea to air.

In the sea water, just below the surface (level 0-) :

- The upwelling flux, $F_{total}^{0-,up}$, is due to the scattering of light in the water.
- The downwelling flux, $F_{total}^{0-,down}$, is due to the air/sea transmission of the incident atmospheric flux and to the downward reflection on the sea/air interface of the upwelling diffuse marine light.

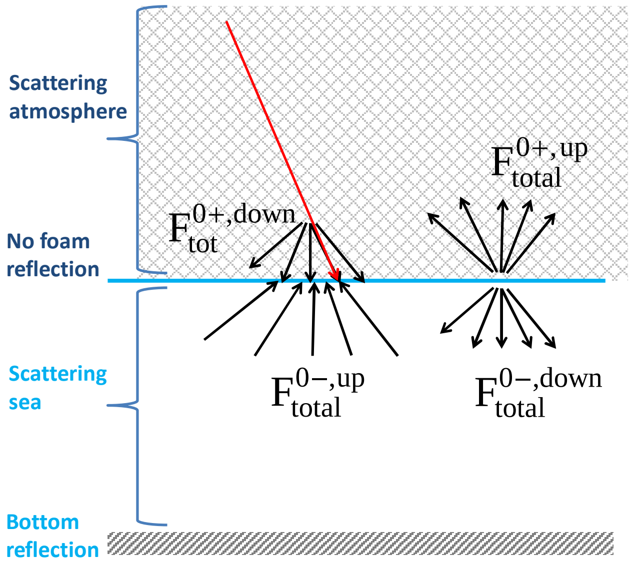


Figure 15 : Fluxes on the air/sea interface

The energy of the incident fluxes reaching the surface interface from the atmosphere as well as from the sea must be distributed in the reflected and transmitted fluxes. Then, we must check :

$$\boxed{F_{total}^{0+,down} + F_{total}^{0-,up} = F_{total}^{0+,up} + F_{total}^{0-,down}}$$

5.2.1 Conditions of the simulations

The conditions of the simulations are the same as for the previous case, except for:

- Solar zenith angle: 10°, 30° and 50°.
- Wavelength: 443 nm

- 40 or 80 gauss angles are used to analyse the sensitivity of calculations to the gauss quadrature.
- Atmospheric scattering by molecules (no aerosols): Rayleigh optical thickness = 0.23.
- Sea depth: 5 m.
- Wind velocity at surface level: 0 (flat sea), 0.5, 1, 2, 5 and 7 m/s.

5.2.2 Results

Table 15 shows the results.

By using 80 Gauss angles, we notice the consistency of **the fluxes conservation is better than 0.3% for a rough sea**, for a solar zenith angle in the range of 10° to 50°.

In case of using only 40 Gauss angles, the accuracy can be strongly degraded for the lowest wind velocities (smaller than 2 m/s), mainly for low solar zenith angles.

	40 μ_{GAUSS}						80 μ_{GAUSS}					
$\theta_S = 10°$	Wind m/s						Wind m/s					
	0	0,5	1	2	5	7	0	0,5	1	2	5	7
$F_{total}^{0+,down}$	2,783	2,787	2,787	2,787	2,786	2,786	2,783	2,788	2,787	2,787	2,786	2,786
$F_{total}^{0+,up}$	0,103	0,100	0,101	0,101	0,099	0,098	0,103	0,102	0,101	0,101	0,099	0,098
$F_{total}^{0-,down}$	2,707	2,373	2,615	2,712	2,723	2,725	2,714	2,718	2,718	2,719	2,723	2,725
$F_{total}^{0-,up}$	0,031	0,028	0,030	0,032	0,032	0,032	0,032	0,032	0,032	0,032	0,032	0,032
$F_{total}^{0+,up}$ + $F_{total}^{0-,down}$	**2,809**	**2,473**	**2,716**	**2,813**	**2,822**	**2,823**	**2,817**	**2,820**	**2,820**	**2,820**	**2,822**	**2,823**
$F_{total}^{0+,down}$ + $F_{total}^{0-,up}$	**2,815**	**2,815**	**2,818**	**2,818**	**2,818**	**2,818**	**2,815**	**2,819**	**2,819**	**2,819**	**2,818**	**2,818**
Absolute difference	-0,005	-0,342	-0,101	-0,006	0,004	0,005	0,002	0,001	0,001	0,001	0,004	0,005
Relative diff (%)	-0,19	-12,15	-3,59	-0,20	0,13	0,18	0,07	0,02	0,02	0,05	0,13	0,18

θ_S = 30°	Wind m/s						Wind m/s					
	0	0,5	1	2	5	7	0	0,5	1	2	5	7
$F_{total}^{0+,down}$	2,414	2,419	2,418	2,418	2,417	2,417	2,414	2,418	2,418	2,418	2,417	2,417
$F_{total}^{0+,up}$	0,094	0,094	0,093	0,093	0,092	0,091	0,094	0,094	0,093	0,093	0,092	0,091
$F_{total}^{0-,down}$	2,342	2,475	2,373	2,354	2,359	2,361	2,351	2,354	2,355	2,356	2,359	2,361
$F_{total}^{0-,up}$	0,029	0,030	0,029	0,029	0,029	0,029	0,029	0,029	0,029	0,029	0,029	0,029
$F_{total}^{0+,up} + F_{total}^{0-,down}$	**2,437**	**2,569**	**2,466**	**2,447**	**2,450**	**2,452**	**2,446**	**2,448**	**2,448**	**2,448**	**2,450**	**2,452**
$F_{total}^{0+,down} + F_{total}^{0-,up}$	**2,443**	**2,449**	**2,447**	**2,447**	**2,446**	**2,446**	**2,443**	**2,447**	**2,447**	**2,447**	**2,446**	**2,446**
Absolute difference	-0,007	0,120	0,018	0,000	0,004	0,006	0,002	0,000	0,001	0,002	0,004	0,006
Relative diff (%)	-0,27	4,91	0,75	0,01	0,16	0,23	0,10	0,02	0,03	0,06	0,16	0,23

θ_S = 50°	Wind m/s						Wind m/s					
	0	0,5	1	2	5	7	0	0,5	1	2	5	7
$F_{total}^{0+,down}$	1,725	1,731	1,731	1,731	1,731	1,732	1,725	1,731	1,731	1,731	1,731	1,732
$F_{total}^{0+,up}$	0,091	0,091	0,091	0,091	0,091	0,091	0,091	0,091	0,091	0,091	0,091	0,091
$F_{total}^{0-,down}$	1,649	1,671	1,664	1,665	1,668	1,669	1,660	1,664	1,664	1,665	1,668	1,670
$F_{total}^{0-,up}$	0,023	0,023	0,023	0,023	0,023	0,023	0,023	0,023	0,023	0,023	0,023	0,023
$F_{total}^{0+,up} + F_{total}^{0-,down}$	**1,740**	**1,762**	**1,755**	**1,755**	**1,759**	**1,760**	**1,751**	**1,754**	**1,755**	**1,755**	**1,759**	**1,761**
$F_{total}^{0+,down} + F_{total}^{0-,up}$	**1,748**	**1,754**	**1,754**	**1,754**	**1,754**	**1,755**	**1,748**	**1,754**	**1,754**	**1,754**	**1,754**	**1,755**
Absolute difference	-0,008	0,008	0,001	0,002	0,004	0,006	0,003	0,000	0,001	0,002	0,004	0,006
Relative diff (%)	-0,46	0,43	0,04	0,09	0,24	0,32	0,17	0,03	0,05	0,09	0,24	0,32

Table 15 : Flux conservation budget at air/sea interface.
Simulation at 443-nm, for a wind velocity from 0 to 7 m/s, atmospheric and marine scattering environments (molecules) without foam and for a black sea bottom.
40 or 80 Gauss angles. 3 solar zenith angles: 10, 30 and 50°.

5.3 Conclusion

The validation of OSOAA has been performed both on the stokes parameters (I,Q,U) radiance fields by comparison to the JC's code (Jacek Chowdhary's code) and on the flux conservation at the air/sea interface.

The consistency of OSOAA simulations for a rough sea with respect to the JC's code is better than 0.4×10^{-3} of normalized radiance for the intensity. The comparison between both code is lower than 0.1×10^{-3} for the polarization parameters Q and U. The relative differences do not exceed 0.8%, except for the parameters Q and U when the directions of observation corresponds to the case for which the degree of polarization is very close to zero (in this latter case, the relative difference is meaningless).

Regarding the flux conservation at the air/sea interface, the uncertainty is lower than 0.3% for a rough sea for a solar zenith angle in the range of 10° to 50° and by using an appropriated Gauss quadratre (80 Gauss angles).