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SUCCESSIVE ORDERS OF SCATTERING RADIATIVE TRANSFER CODE - INCLUDING THE GASEOUS ABSORPTION

SOS-ABS

USER MANUAL

Reference : SOS-ABS-MU
Version 1.0 - 09/11/2023

The SOS-ABS code is on CNES GitHub at :
https://github.com/CNES/RadiativeTransferCode-SOS

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1. INTRODUCTION

Authors:

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

The approach to modelling the gaseous transmissions was established in collaboration with the **LOA** laboratory (Pr. Phillipe Dubuisson and Pr. Jérôme Riedi). The CKD coefficients were calculated by the **HYGEOS** company (Dr. Mathieu Compiègne).

The specification and implementation for SOS-ABS of the absorption and scattering coupling effect were made by **CS GROUP France** (Dr. Lafrance Bruno and Dr. Xavier Lenot).

This document is the user manual for the SOS-ABS code.

It presents the software installation (chapter §2) and the operating mode (chapters §3 and §4). The various input and output files are presented in chapter §5. The current chapter introduces the model and gives the scientific references.

1.1 What is the SOS-ABS radiative transfer code?

The SOS-ABS code (Successive Orders of Scattering method coupled with the gaseous ABSorptions) is a 1D plan parallel radiative transfer code simulating the polarized radiance of the {Earth surface – atmosphere} system, including the coupling effect of gaseous absorption. It works for the reflective spectral domain, from 2500 to 27500 cm^{-1} (0.364 μm to 4 μm), under clear sky conditions.

It is an heritage of the original Successive Orders of Scattering method from the LOA laboratory [Deuze et al, 1989, - RD4] [Lenoble et al., 2007 - RD9].

The SOS-ABS model includes the initial features and improved methods. SOS-ABS allows simulating:

- **Atmospheric profiles**:
  For the characterization of the atmosphere, the user can define the molecular and aerosol optical thickness.
  The user can also define the amount of gas among ozone (O_3), water vapour (H_2O), carbon dioxide (CO_2) and methane (CH_4). The dioxygen (O_2), nitrous oxide (N2O), nitrogen dioxide (NO_2) and carbon monoxide (CO) are also considered. The vertical distribution is based on typical profiles (Tropical, Middle Latitude Summer or Winter, South Arctic Summer or Winter, US Standard), or given by a user's atmospheric profile.

- **Aerosol models:**

  A wide variety of aerosol size distribution is available in the SOS-ABS 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, pre-calculated WMO [WMO, 1986 - RD16] or Shettle & Fenn models [Shettle and Fenn, 1979 - RD15]) can be used. It is also possible to simulate a combination of various mono-modal modes, as defined by the user, which is compliant with the use of CAMS data [RD1].

  Users can also use their own aerosol phase function and radiative properties.

- **Surface reflection models:**

  The reflection of the direct solar beam and of the diffuse light on the surface is considered for both land and water surfaces. Over land, a Lambertian target can be simulated as well as the Roujean's BRDF model [Roujean et al., 1992 - RD14]. The polarization of the surface can be considered too with the Rondeaux's model [Rondeaux and Herman, 1991 - RD13], the Bréon's model [Bréon et al., 1995 - RD2] or the Maignan's model [Maignan et al., 2009 - RD10]. Over a sea surface, the air / sea interface can be modelled either for a flat surface or by considering the sea roughness defined by the wind speed and the correlated waves [Cox and Munk, 1954 - RD3].

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

By default, SOS-ABS provides the upward radiance field at TOA and the downward radiance at ground level. However, it is also possible to get the upward and downward radiance, in term of intensity and polarized light, for any given altitude in the atmosphere.

1.2 Reference documents

Ref	Document
RD1	A. Bozzo, S. Remy, A. Benedetti, J. Flemming, P. Bechtold, M.J. Rodwell and J.-J. Morcrette, « Implementation of a CAMS-based aerosol climatology in the IFS », ECMWF Technical memorandum, April 2017, doi 10.21957/84ya94mls
RD2	Bréon F. M., D. Tanre, P. Lecomte and M. Herman, "Polarized Reflectance of Bare Soils and Vegetation – Measurements and Models", *IEEE T. Geosci. Remote*, 33, 487–499, 1995.
RD3	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.

RD4	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.
DR5	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.
DR6	Hansen J. and Travis L., "Light scattering in planetary atmospheres", *Space Sci. Rev*., Vol. 16., pp. 527-610, 1974.
DR7	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
RD8	Lacis, A.A., and V. Oinas, A description of the correlated k-distribution method, *J. Geophys. Res.,* 96, 9027-9064, 1991.
RD9	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.
RD10	Maignan F., F. M. Breon, E. Fedele and M. Bouvier, "Polarized reflectances of natural surfaces: Spaceborne measurements and analytical modeling", *Remote Sens. Environ.*, 113, 2642–2650, 2009.
DR11	Mie G., Beiträge zur Optik trüber Medien, speziell kolloidaler Metallösungen, *Annalen der Physik*, vol. 330, Issue 3, pp.377-445, 1908.
DR12	J. Perbos," Modèle radiomètrique d'effets atmosphériques et logiciel associé (ATMLIB),". Version I, Division traitement de l'image, CNES, Toulouse, p. 52, December 1982.
RD13	Rondeaux G. and M. Herman, « Polarization of light reflected by crop canopies », *Remote Sens. Env*., no. 38, pp. 63-75, 1991.
RD14	Roujean J.L., M. Leroy, and P.Y. Deschamps, « A bidirectional reflectance model of the Earth surface for the correction of remote sensing data », *J. Geophys.* Res., no. 97, pp. 20455-20468, 1992.
RD15	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.
RD16	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 Acronyms

The acronyms used in this document are listed below.

Acronym	Signification
AOT	Aerosol optical thickness
BRDF	Bidirectional Reflectance Distribution Function
BPDF	Bidirectional Polarization Distribution Function
CAMS	Copernicus Atmosphere Monitoring Service
CNES	Centre National d'Etudes Spatiales (Toulouse, France)
CS Group	Communication & Systems Group
IOP	Inherent Optical Properties
LOA	Laboratoire d'Optique Atmosphérique (Villeneuve d'Ascq, France)
LND	Log Normal Distribution
Ppmv	Parts Per Million by Volume
SOS	Successive Orders of Scattering
TOA	Top Of Atmosphere

2. SOFTWARE INSTALLATION

2.1 SOS-ABS package

The SOS-ABS arborescence must be deployed on the user account.

The files are structured in the following sub-directories:

- **src**: contains the source codes in Fortran 77.

SOS_ABS_MAIN.F	Main program of SOS-ABS. Manages the simulation parameters and the software run from a command line.
SOS_PROC.F	This procedure checks the simulation parameters and executes the sequence of the various code modules. It is the procedure used with the binding Python.
SOS_ANGLES.F	Manages the definition of zenith angles and expansion orders.
SOS_AEROSOLS.F	Computes the aerosol radiative properties.
SOS_MIE.F	Computes MIE calculations of radiative properties as a function of the size parameter.
SOS_SURFACE.F	Manages the calculation of surface reflection properties: BRDF / BPDF matrices.
SOS_NOM_FIC_SURFACE.F	Manages file names for BRDF/BPDF matrices.
SOS_ROUJEAN.F	Computes the reflection from Roujean's BRDF model.
SOS_GLITTER.F	Computes the sun-glint reflection on sea waves.
SOS_SURFACE_BPDF.F	Computes the BPDF from Rondeaux-Herman, Bréon or Maignan's models.
SOS_PREPA_ABSPROFILE.F	Prepares the absorption profile: CKD coefficients, gaseous concentration profile (50 layers).
SOS_SUB_TRS.F	Computes the absorption coefficients from the CKD model for a given pressure and temperature.
SOS_ABSPROFILE.F	Computes the profile of the gaseous optical thickness (50 layers) for a given term (exponential) of the CKD expansion.
SOS_PREPA_OS.F	Prepares the parameters for a single radiative transfer calculation
SOS_PROFIL.F	Computes the profile of optical thickness, combining the molecules and aerosols scattering and the gaseous absorption. It gives the relative proportion of the molecular optical thickness and of the aerosols optical thickness with respect to the total optical thickness. The vertical profile is defined at SOS resolution.

SOS.F	Runs a single radiative transfer calculation. The procedure adjusts the optical thickness profile to a truncation of the aerosol phase function.
SOS_OS.F	Computes a radiative transfer calculation for a given surface model, a given aerosol model and a given profile of optical thickness and relative proportion of scattering for molecules and aerosols. Results are given as a Fourier series expansion.
SOS_AGGREGATE.F	Manages the ponderation of the radiative transfer calculation for each CKD term (each exponential) and agglomerates the results to calculate the global radiance.
SOS_TRPHI.F	Computes the recombination of the radiance to a given azimuth angle.

- **gen**: contains the Makefile used to compile the source codes and get the executable file SOS_ABS.exe

- **exe**: contains the executable code and a demo launch script.

- **inc**: contains the file SOS.h which lists all the constant parameters (see section 0) shared by the different source codes. It specifies the names of predefined physical data files (WMO and Shettle & Fenn aerosol models). It provides default values of physical parameters and of inner array size dimensions. This file also defines a set of thresholds used for computations.

- **fic**: contains data files required for the processing:
    - Aerosol data files obtained from WMO and Shettle & Fenn models:
        - DataWMO,
        - DataSF, IRefrac_LR, IRefrac_LU, IRefrac_OM, IRefrac_SR, IRefrac_SU.
    - SO2-NO2 file: profile for SO2 and NO2 components (in ppmv).
    - COEFF_CKD/1cmm1/coef*, COEFF_CKD/5cmm1/coef*, COEFF_CKD/10cmm1/coef* :

      files of CKD coefficients at 1, 5 or 10 cm^{-1} spectral resolution for CH_4, CO, CO_2, H_2O, N_2O, NO_2, O_2 and O_3.

- **doc**: contains the documentation.

- **binding**: contains the procedure to compile the code sources and generate the shared library sos.so file (giving access to the sos_proc routine for a python code).

2.2 Compilation

The SOS-ABS code can be executed from a command line or from a python code via a binding.
The compilation process is specific to a command-line use or a use from python code.

The compilation was tested with **gcc version 10.2.0** and **Python version 3.10.9** on Linux computer.

2.2.1 Defining the SOS_ABS_ROOT environment variable

The user must define the *environment variable* **SOS_ABS_ROOT** which points on the SOS_ABS main folder path.

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

2.2.2 Compilation process for a use by command line

Let's move from the current directory to "**gen**" (> *cd $SOS_ABS_ROOT/gen*) and run the makefile:

> ***make –f Makefile.gfortran***

Upon completion, one can find:

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

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

2.2.3 Compilation process for a use of SOS-ABS from a python code

The "**binding**" directory **($SOS_ABS_ROOT/binding**) contains the compilation script, called "compilation_f2py". Let's execute the script:

> ***. ./compilation_f2py***

Upon completion, one can find in the **sos.os** file in the "binding" directory.

3. OPERATING MODE FROM COMMAND LINES

This chapter describes the procedure to execute a simulation with SOS_ABS, using command lines.

The processing parameters are divided into two set of parameters:

- Physical parameters specific to the simulation, listed in the example of command line script **runSOS-ABS_demo.ksh** (located in **$SOS_ABS_ROOT/exe/**).
- Dimensioning parameters, predefined physical parameters and threshold values assigned in the include file **SOS.h** (located in **$SOS_ABS_ROOT/inc/**). Those are common for a use by command lines or by binding Python.

3.1 Simulation parameters

The simulation parameters can be distinguished in 6 sets of parameters:

- General parameters: see §3.1.1.
- Atmospheric profile parameters: see §3.1.2, page 14.
- Aerosol parameters: see §3.1.3, page 20.
- Surface parameters: see §0, page 29.
- Angle calculation parameters: see §3.1.5, page 32.
- Selection of expected outputs: see §3.1.6, page 33.

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

The command file can be written by the user (see example in section §0, page 36).

> **Note**:
> A given simulation requires defining only the useful input parameters. The useless input parameters (i.e, those who are not concerned by the options selected for the given simulation) should not be defined. However, note that if a useless parameter is still defined, it will not be taken into account by the software during the run.
>
> Note also that if a useful parameter is missing, the software stops processing the run and the user is informed about the name of the parameter that should be defined.

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 from the devoted constant value in the file SOS.h (located in the directory $SOS_ABS_ROOT/inc).
- **Optional (O)**: the definition of this parameter is optional.
- **Conditional (C)**: the definition of this parameter is required to complete the information of another parameter.

3.1.1 General parameters

The **definition of the working folder** for the SOS-ABS computations is ensured by the keyword **-SOS_Main.ResRoot**. All the output files and log files will be located in this working folder in specific sub-directories (SOS, LOG) which are automatically created when performing a simulation.

The **wavelength for the radiance calculations** is defined by the keyword **-SOS_Main.Wa**. Radiative parameters are defined for this wavelength, such as the aerosol refractive indices, the molecular optical thickness or surface albedo.

The **solar zenith angle** is defined by the keyword **-ANG.Thetas**.

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

Table 1 : General parameters
Magenta words correspond to the names of the python binding parameters

Parameter	Definition	R/O
-SOS_Main.ResRoot **resroot**	Working folder for the SOS-ABS computations (complete path) *String (SOS_LENDIR characters max)*	**R**
-SOS_Main.Wa **wa_simu**	Wavelength for radiance simulation (µm) *Float*	**R**
-ANG.Thetas **tetas**	Solar zenith angle in degrees (0 < thetas < 90°) *Float*	**R**
-SOS_Main.Log **ficmain_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**

3.1.2 Atmospheric profile definition

The SOS-ABS model needs the profile of scattering and extinction optical thickness from the surface to TOA. It is not generated versus the altitude but versus the optical thickness, which is much more convenient for radiative transfer calculations (Figure 1).

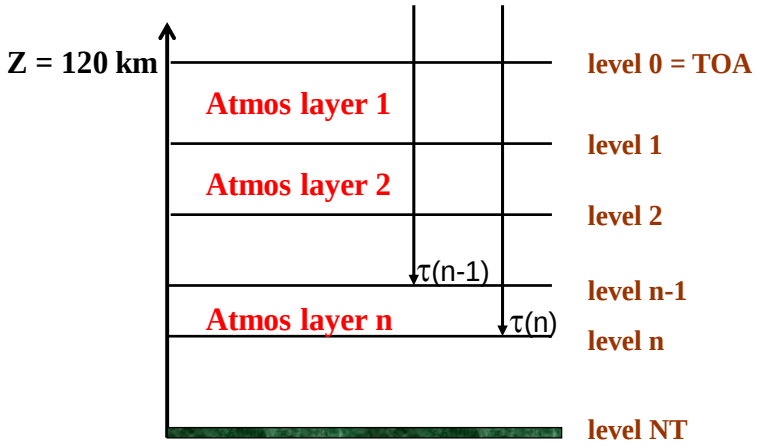

Figure 1 : Discretization of the atmospheric profile

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

The atmospheric profile is automatically calculated by SOS-ABS from parameters characterizing the vertical distribution of particles (molecules, aerosols and absorbing gas).

3.1.2.1 Aerosols and molecules

Molecule optical thickness:

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:

$$\tau_{mol}(z) = \tau_{mol}^{surf} \times \exp(-z / h_{mol}) \quad (1)$$

The molecular optical thickness at ground level τ_{mol}^{surf} is provided by the user (**-AP.MOT**) or calculated from the atmospheric pressure (**-AP.Psurf**) by the following CNES formulation [DR12]:

$$\tau_{mol}^{surf} = \frac{P}{P_0} \times \left(\frac{84{,}35}{\lambda^4} + \frac{-1{,}225}{\lambda^5} + \frac{1{,}4}{\lambda^6} \right) \times 10^{-4} \quad (2)$$

where

- λ is the wavelength (in µm) **–SOS_Main.Wa**
- P is the atmospheric pressure (in mb) **–AP.Psurf**
- P_0 is the standard atmospheric pressure (given by the parameter CTE_HT_STD_PSURF in the SOS.h file: 1013 mb).

Aerosol optical thickness:

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

$$\tau_{aer}(\lambda, z) = \tau_{aer}^{surf}(\lambda) \times \exp(-z / h_{aer}) \quad (3)$$

where

- h_{aer} is the aerosol scale height (in km) **–AP.AerHS.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:

  $$\tau_{aer}^{surf}(\lambda) = \tau_{aer}^{surf}(\lambda_{ref}) \times \frac{\tilde{\sigma}_{aer}^{ext}(\lambda)}{\tilde{\sigma}_{aer}^{ext}(\lambda_{ref})} \quad (4)$$

  The extinction coefficients are calculated from the aerosol model parameters.

In this case, the parameter **–AP.AerProfile.Type** is set to 1.

The user can also simulate an aerosol layer (as a homogeneous mixture of molecules and aerosols) between two pure molecular layers, by setting **-AP.AerProfile.Type** to 2 and by defining the altitudes at the edge of the layer **-AP.AerLayer.Zmin** and **-AP.AerLayer.Zmax** in km.

Note: Currently, this simulation case is only available without taking gaseous absorption into account.

Table 2.a : Aerosol and molecule parameters for the atmospheric profile definition
Magenta words correspond to the names of the python binding parameters

Parameter	Definition	
AP.Log **ficprofil_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**
Aerosols and molecules profile parameters		
AP.AerProfile.Type **iprofil**	Type of the output profile: 1 : profile only defined by height scales 2 : profile defined with 3 distinct layers : (no gas absorption) molecules, molecules + aerosols, molecules *Integer*	**R**
Molecules		
AP.Psurf **psurf**	Atmospheric pressure at surface level in mbar. Default value (in SOS.h): **CTE_HT_STD_PSURF**	**D**
AP.MOT **tr**	Molecular optical thickness for the wavelength of radiance simulation *Float*	**O**
If AP.MOT ≥ 0		
AP.HR **hr**	Height scale of the molecular profile (km). *Float*	**C**
Aerosols		
AER.AOTref **aot_ref**	Aerosol optical thickness for the reference wavelength *Float*	**R**
If AER.AOTref > 0.		
AER.Waref **waref_aot**	Reference wavelength (µm) for the aerosol optical thickness (AER.AOTref) *Float*	**C**
If AP.AerProfile.Type = 1 & AER.AOTref ≥ 0		
AP.AerHS.HA **ha**	Height scale of the aerosol profile (km). *Float*	**C**
If AP.AerProfile.Type = 2		
AP.AerLayer.Zmin	Minimum layer altitude of the mixture molecules + aerosols (km)	**C**
AP.AerLayer.Zmax **zmin, zmax**	Maximum layer altitude of the mixture molecules + aerosols (km) *Float*	**C**

3.1.2.2 Absorbing gases

The SOS-ABS code considers the gaseous absorption, as a coupling effect between light scattering and absorption, for the following gas impacting the spectral range between 0.364 and 4.0 μm:

- ✓ Ozone (O_3)
- ✓ Water vapor (H_2O)
- ✓ Dioxygen (O_2)
- ✓ Carbon dioxide (CO_2)
- ✓ Methane (CH_4)
- ✓ Nitrous oxide (N_2O)
- ✓ Nitrogen dioxide (NO_2)
- ✓ Carbon monoxide (CO)

It is possible to exclude some species by setting to 0 the associated constant in the SOS.h file (requiring a new compilation of the software): CTE_ABS_H2O, CTE_ABS_CO2, CTE_ABS_O3, CTE_ABS_N2O, CTE_ABS_CO, CTE_ABS_CH4, CTE_ABS_O2 or CTE_ABS_NO2 (see section §0).

There are three ways of defining the gas profile:

- **Predefined standard atmospheric profiles: -AP.AbsProfile.Type 1 to 6**

  Predefined atmospheric profiles (gas concentration, temperature and pressure) are available. The user can select the profile with the parameter **-AP.AbsProfile.Type**. Table 3 lists the proposed profiles and shows their default amount of ozone, water vapor, carbon dioxide and methane.

Table 3 : Default value of amount of O_3, H_2O, CO_2 and CH_4 depending on the selected atmospheric profile. The profile number corresponds to the parameter -AP.AbsProfile.Type

N°	Name of the profile	H_2O (g/cm^2)	O_3 (Dobsons)	CO_2 (ppmv)	CH_4 (ppmv)
1	Tropical	4.068	280.95	330	1.7
2	Mid-Latitude Summer	2.906	333.12		
3	Mid-Latitude Winter	0.853	376.85		
4	Sub-Arctic Summer	2.080	346.57		
5	Sub-Arctic Winter	0.417	374.78		
6	US Standard Atmosphere 1962	1.417	343.03		
7	No absorption	0	0	0	0

- **Predefined standard atmospheric profiles with gas amount weighting:**

  In replacement of the default values, the total ozone and water vapour amounts can be defined by the user (value of the total column amounts), such as the carbon dioxide and methane (value of concentration at surface level). In this case, the default profile is adjusted to the user's values (see Table 4).

Table 4 : Parameters to define the gas amount

Gas	Amount definition	Unit	Keyword
Ozone (O_3)	Total column amount	Dobson	**-AP.O3**
Water vapor (H_2O)	Total column amount	g/cm^2	**-AP.H2O**
Dioxygen (O_2)			None
Carbon dioxide (CO_2)	Concentration at surface level	ppmv	**-AP.CO2**
Methane (CH_4)	Concentration at surface level	ppmv	**-AP.CH4**
Nitrous oxide (N_2O)			None
Nitrogen dioxide (NO_2)			None
Carbon monoxide (CO)			None

- **Predefined standard atmospheric profiles: -AP.AbsProfile.Type 0**

  The users can also prefer using their own gas profiles, provided by a formatted file defined by the parameter **-AP.AbsProfile.UserFile**, associated to **-AP.AbsProfile.Type** 0. The content and format are described in section §5.1.2, from page 50.

The modelling of the transmittance by gas absorption is based on the CKD method [RD8]. Therefore, in addition to profile information, the introduction of gas absorption requires to define the spectral resolution to be considered for the absorption data. This is defined by the **-AP.SpectralResol** parameter, whose value can be 1, 5 or 10 cm^{-1}.

The finest way to apply the CKD method requires to calculate the radiance from each term of the CKD expansion. Therefore, it is necessary to estimate the gas transmittance and the resulting optical thickness profile to calculate each elementary radiance of the CKD expansion. The total radiance is obtained by combining the elementary radiance estimates, taking into account a weighting for each expansion term. Depending on the number of expansion terms, this calculation is more or less time consuming.

Another possibility is to only calculate the gas transmittance based on the CKD method and the resulting optical thickness profile before performing a single radiance calculation. The advantage of this method is to be faster than the fine CKD approach, with results accurate and close to those of the fine CKD method for moderate absorption bands. On the opposite, the approximate CKD method is not suitable for strong absorption bands. In this case, the fine CKD method is recommended.

The finest CKD calculation is realised by setting **-SOS.AbsModeCKD** to 1, while the approximate CKD calculation is applied when **-SOS.AbsModeCKD** is 2.

Table 2.b : Gas parameters for the atmospheric profile definition
Magenta words correspond to the names of the python binding parameters

Gas absorption parameters		
AP.AbsProfile.Type **absprofil**	Type of gas profile: 0 : User profile 1 : Tropical profile 2 : Middle Latitude Summer profile 3 : Middle Latitude Winter profile 4 : South Arctic Summer profile 5 : South Artic Winter profile 6 : USST62 profile 7 : No gas absorption *Integer*	**R**
If AP.AerProfile.Type = 1 & AP.AbsProfile.Type ≠ 7		
AP.SpectralResol **nustep**	Spectral resolution for gas absorption data (in cm^{-1}) (1, 5 ou 10 cm^{-1}) *Integer*	**C**
SOS.AbsModeCKD **imode_ckd_calcul**	Option for the application of the CKD method: 1 : Fine modelling of absorption / scattering coupling 2 : Simplified modelling of the absorption effects (use of the CKD method for a single estimate of the absorption optical thickness). *Integer*	**C**
AP.H2O **h2o**	Water vapor content (g/cm^2). If not defined, the value is that of the selected atmospheric profile. *Float*	**O**
AP.O3 **o3**	Ozone content (Dobson). If not defined, the value is that of the selected atmospheric profile. *Float*	**O**

AP.CO2 **co2**	Carbon dioxide concentration at surface level (in ppmv) If not defined, the value is that of the selected atmospheric profile. *Float*	**O**
AP.CH4 **ch4**	Methane concentration at surface level (in ppmv) If not defined, the value is that of the selected atmospheric profile. *Float*	**O**
If AP.AbsProfile.Type = 0		
AP.AbsProfile.UserFile **ficabsprofil**	User's file defining the gas profiles (complete path) *String (CTE_LENFIC2 characters max)*	**C**

3.1.3 Aerosol parameters

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

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

Table 5.a : Basic aerosol parameters and type of aerosol model
Magenta words correspond to the names of the python binding parameters

Parameter	Definition	O/ D/C
AER.Log **ficgranu_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 **ficmie_log**	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 **ficgranu**	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 SOS.h): **CTE_DEFAULT_FICGRANU**	**D**

Parameter	Definition	O/ D/C
AER.UserFile **ficuser_aer**	File name for user-precomputed Aerosols radiative properties (full path). Note: The file includes the information relative to phase function truncature. Special requirement: For this specific simulation case, the reference aerosol wavelength (-AER.Waref) and the radiance simulation wavelength (-SOS_Main.Wa) must be equal.	**O**
If AER.AOTref > 0		
AER.DirMie **dir_mie**	Directory for aerosol MIE files storage (complete path) *String (CTE_LENDIR characters max)*	C1
AER.Tronca **itronca_aer**	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**
AER.Model **imod_aer**	Type of aerosol model 0 : Mono-modal 1 : WMO multi-modal 2 : Shettle & Fenn bi-modal 3 : Log-Normal bi-modal 4 : Radiative properties from an external source 5 : Multi-modes model defined by user *Integer*	**C1**

3.1.3.1 Mono-modal size distributions of aerosols

The size distribution of aerosols 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}).

- **Log-Normal size Distribution (LND): -AER.Model 0 -AER.MMD.SDtype 1**

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

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 refractive index of particles is given by its real and imaginary parts for the wavelength of the radiance simulation, respectively set by the parameters **-AER.MMD.MRwa** and **-AER.MMD.Miwa**.

If the aerosol optical thickness (AOT) is given for a different wavelength, the user must define the refractive index for the reference wavelength of the AOT: **-AER.MMD.MRwaref and -AER.MMD.Miwaref**.

- **Junge's law model: -AER.Model 0 -AER.MMD.SDtype 2**

$$\begin{cases} r \le r_{min} : N_{aer}^{Junge}(r) = r_{rmin}^{-\upsilon} \\ r_{min} < r \le r_{max} : N_{aer}^{Junge}(r) = r^{-\upsilon} \\ r > r_{max} : N_{aer}^{Junge}(r) = 0 \end{cases} \quad (6)$$

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 SOS.h file.
- υ : the slope of the Junge's law
  → defined by the user : **-AER.MMD.JD.slope**.

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

Table 5.b : Parameters for mono-modal size distributions of aerosols
Magenta words correspond to the names of the python binding parameters

If AER.Model = 0 : parameters of mono-modal size distributions		
AER.MMD.MRwa **rn_wa**	Real part of the aerosol refractive index for the wavelength of radiance calculation *Float F5.3*	**C2**
AER.MMD.MIwa **in_wa**	Imaginary part of the aerosol refractive index for the wavelength of radiance calculation (negative value) *Float F8.5*	**C2**
AER.MMD.Sdtype **igranu**	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 **lnd_radius_mmd_aer**	Modal radius (µm) of the Log-Normal size distribution *Float*	**C2**
AER.MMD.LNDvar **lnd_lnvar_mmd_aer**	Standard deviation of the Log-Normal size distribution *Float*	**C2**
If AER.MMD.SDtype = 2 : Junge size distribution		
AER.MMD.JD.slope **jd_slope_mmd_aer**	Slope of the Junge's law Warning: 3 is a singular value *Float*	**C2**
AER.MMD.JD.rmin **jd_rmin_mmd_aer**	Minimal radius of the Junge's law (µm)	**C2**
AER.MMD.JD.rmax **jd_rmax_mmd_aer**	Maximal radius of the Junge's law (µm) *Float* Default value (in SOS.h): **CTE_DEFAULT_AER_JUNGE_RMAX**	**D**
If AER.Waref ≠ SOS_Main.Wa		
AER.MMD.MRwaref **rn_waref**	Real part of the aerosol refractive index for the reference wavelength of aerosol properties calculation *Float F5.3*	**C2**
AER.MMD.MIwaref **in_waref**	Imaginary part of the aerosol refractive index for the reference wavelength of aerosol properties calculation (negative value) *Float F8.5*	**C2**

3.1.3.2 WMO aerosol models

The user can select a WMO model by setting **-AER.Model 1**

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 (ratios of dust like, water soluble, oceanic and soot particles with **-AER.WMO.DL**, **-AER.WMO.WS**, **-AER.WMO.OC** and **-AER.WMO.SO** to be set between 0 and 1).

Table 5.c : Parameters for WMO aerosol models
Magenta words correspond to the names of the python binding parameters

If AER.Model = 1 : WMO aerosol model		
AER.WMO.Model **imodele_wmo**	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 **c_wmo_dl**	Volume concentration (between 0 and 1) of "Dust-Like" component *Float*	**C3**
AER.WMO.WS **c_wmo_ws**	Volume concentration (between 0 and 1) of "Water Soluble" component *Float*	**C3**
AER.WMO.OC **c_wmo_oc**	Volume concentration (between 0 and 1) of "OCeanic" component *Float*	**C3**
AER.WMO.SO **c_wmo_so**	Volume concentration (between 0 and 1) of "SOot" component *Float*	**C3**

3.1.3.3 Shettle and Fenn aerosol models

The user can select a Shettle and Fenn model by setting **-AER.Model 2**

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 percent).

These predefined models are based on a mixture of elementary components (Small rural, large rural, small urban, large urban, oceanic particles) for which inherent optical properties have already been calculated.

Table 5.d : Parameters for Shettle and Fenn aerosol models
Magenta words correspond to the names of the python binding parameters

If AER.Model = 2 : Shettle & Fenn aerosol model		
AER.SF.Model **imodele_sf**	Shettle & Fenn model : 1 : Tropospheric 2 : Urban 3 : Maritime 4 : Coastal *Integer*	**C4**
AER.SF.RH **rh**	Percentage of air relative humidity (from 0 to 99%) *Float*	**C4**

3.1.3.4 Bi-modal LND aerosol models

The user can select a bimodal Log-Normal model by setting **-AER.Model 3**

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 mode of particles.

The volume size distribution of bimodal models is given by:

$$\frac{dV(r)}{d\ln r} = \sum_{i=1}^{2} \frac{C_{V,i}}{\sigma_i \sqrt{2\pi}} \times \exp\left[\frac{-\ln^2(r/r_i)}{2\sigma_i^2}\right] \qquad (7)$$

with :

- $C_{V,i}$: the volume concentration for mode i particles (in μm^3 / μm^2).

  → 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.

$$r(\lambda_{ref}) = \frac{\tau_{aer}^{C}(\lambda_{ref})}{\tau_{aer}^{tot}(\lambda_{ref})} \quad (8)$$

→ 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, the code calculates the fine and coarse scattering cross-sections ($\tilde{\sigma}_{sca}^{F}(\lambda_{ref})$, $\tilde{\sigma}_{sca}^{C}(\lambda_{ref})$) and extinction cross-sections ($\tilde{\sigma}_{ext}^{F}(\lambda_{ref})$, $\tilde{\sigma}_{ext}^{C}(\lambda_{ref})$).

The refractive index of particles must be given both for the coarse and fine modes, using parameters:

-AER.BMD.CM.MRwa, **-AER.BMD.CM.MIwa**, **-AER.BMD.FM.MRwa** and **-AER.BMD.FM.MIwa**.

If the total AOT is given for a reference wavelength, then the refractive index must be defined for this wavelength too, using the parameters: **-AER.BMD.CM.MRwaref**, **-AER.BMD.CM.MIwaref**, **-AER.BMD.FM.MRwaref** and **-AER.BMD.FM.MIwaref**.

Table 5.e : Parameters for bi-modal LDN aerosol models
Magenta words correspond to the names of the python binding parameters

If AER.Model = 3 : Log-Normal bi-modal aerosol model		
AER.BMD.VCdef **mode_param_bilnd**	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**
If AER.BMD.VCdef = 1 : user-defined volume concentrations		
AER.BMD.CoarseVC **user_cv_coarse**	User volume concentration of the "LND coarse mode" *Float*	**C3**
AER.BMD.FineVC **user_cv_fine**	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 **rtauct_waref**	User value of the ration AOT_coarse / AOT_total for the aerosol reference wavelength. *Float*	**C3**
Coarse mode LND parameters		
AER.BMD.CM.MRwa **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 **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 **bmd_cm_rmodal**	Modal radius of the "LND coarse mode" (µm) *Float*	**C2**
AER.BMD.CM.SDvar **bmd_cm_var**	Standard deviation of the "LND coarse mode" *Float*	**C2**
If AER.Waref ≠ SOS_Main.Wa		
AER.BMD.CM.MRwaref **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 **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 **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 **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**
AER.BMD.FM. SDradius **bmd_fm_rmodal**	Modal radius of the "LND fine mode" (µm) *Float*	**C2**
AER.BMD.FM.SDvar **bmd_fm_var**	Standard deviation of the "LND fine mode" *Float*	**C2**

If AER.Waref ≠ SOS_Main.Wa		
AER.BMD.FM.MRwaref **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 **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**

3.1.3.5 Aerosol data from external sources

Table 5.f : Parameters for aerosol data from external sources
Magenta words correspond to the names of the python binding parameters

If AER.Model = 4 : Phase functions from an external source		
AER.ExtData **ficexdata_aer**	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 (-SOS_Main.Wa) must be equal. *String (CTE_LENFIC2 characters max)*	**C2**
If AER.Model = 5 : Multi-modes model defined by the user		
AER.DefMixture **ficmixture_aer**	User's file (complete path) defining the mixture of aerosol modes. *String (CTE_LENFIC2 characters max)*	**C2**

The SOS-ABS model can also ingest aerosol information from external sources:

- **IOP from external source:** **-AER.Model 4**

  The user can provide the aerosols optical properties in a file defined by **-AER.ExtData**.

  This can be useful for simulating an aerosol model that is not implemented in the SOS-ABS model, for instance non-spherical particles for which the IOP would be available.

  The content and format of this file is described in section §5.1.3, page 52.

- **Multi-modes models:** **-AER.Model 5**

  The user can also define a more complex mixture of particles by combining a set of different modes. This is useful to apply CAMS aerosol models.

  The aerosol parameters are given in a file located by **-AER.DefMixture**.

  The content and format of this file is described in section §5.1.5, page 55.

3.1.4 Surface parameters

The SOS-ABS code can simulate various surface reflection models: a sea surface with or without waves, a lambertian land surface, or a land surface with a direction-dependent reflection model for intensity (BRDF) and polarisation (BPDF).

The choice of the surface model is defined by the parameter **-SURF.Type**.

Over water, the surface can be considered as :

- A flat surface, with a modelling of the Fresnel reflection.
- A rough surface (sunglint case), by simulating the waves shape correlated to the wind velocity by the Cox & Munk model [RD3]) and the reflection properties of wave facets (depending on the water refractive index according to the Fresnel's law).

The refractive index of the water (relative to air) is defined with **-SURF.Ind**. The wind velocity at surface level is given by **-SURF.Glitter.Wind**.

Over land, the surface model can be:

- A **Lambertian surface**, with the surface albedo given by the parameter **-SURF.Alb.**
- a vegetation cover or of a bare land according to the **Roujean's BRDF model** [RD14]

$$\rho_R(\theta_1,\theta_2,\phi) = k_0 + k_1 \times \rho_1(\theta_1,\theta_2,\phi) + k_2 \times \rho_2(\theta_1,\theta_2,\phi) \quad (9.a)$$

with

$$\rho_1(\theta_1,\theta_2,\phi) = \frac{1}{2\pi}\left[(\pi-\phi)\cos\phi + \sin\phi\right].\tan\theta_1.\tan\theta_2 - \frac{1}{\pi}\times\left[\tan\theta_1 + \tan\theta_2 + \sqrt{\tan^2\theta_1 + \tan^2\theta_2 - 2.\tan\theta_1.\tan\theta_2.\cos\phi}\right] \quad (9.b)$$

and $$\rho_2(\theta_1,\theta_2,\phi) = \frac{4}{3\pi}.\frac{1}{\cos\theta_1 + \cos\theta_2}\times\left[\left(\frac{\pi}{2}-\xi\right).\cos\xi + \sin\xi\right] - \frac{1}{3} \quad (9.c)$$

where ξ is the phase angle defined by: $\cos\xi = \cos\theta_1 \times \cos\theta_2 + \sin\theta_1 \times \sin\theta_2 \times \cos\phi$ (10)

Only 3 parameters (k_0, k_1, k_2) are required. They are given by the user, depending on the nature of the surface. Their values must have a dimension consistent with a reflectance simulation.

Warning:
The **Roujean's paper** [RD14] provides values for the parameters **k_0, k_1 and k_2**, expressed **in percent of reflectance**, for different types of vegetation coverages. **For the SOS code these parameters must be 100 times smaller**.

For instance, the coefficients for a « Plowed field » listed in Table 1 of [RD14] are: k_0=24.3, k_1=7.3 and k_2=64.2. To set the command file of SOS-ABS, one must introduce: k_0=0.243, k_1=0.073 and k_2=0.642.

- **A polarized BPDF model**
  - The Rondeaux's model allows to simulate vegetation polarisation [RD13],
  - The **Bréon's model** which is defined for polarisation of bare surfaces [RD2]
  - The Maignan's Model over vegetation or bare soils [RD10]

Incidence angle ↓ Refractive index ←

$$R_p^{Rondeaux}(\theta_S, \theta_V) = \frac{Fp(\alpha_I, n)}{4(\mu_S + \mu_V)} \leftarrow \mu = cos\ \theta$$

$$R_p^{Bréon}(\theta_S, \theta_V) = \frac{Fp(\alpha_I, n)}{4\mu_S\mu_V}$$

$$R_p^{Maignan}(\theta_S, \theta_V) = \frac{C \exp(-tan(\alpha_I)) \exp(-\nu) F_p(\alpha_I, n)}{4(\mu_S + \mu_V)}$$

ν = NDVI
C = ponderation coef

We have chosen the Roujean's BRDF model to simulate the intensity of the polarisation reflection matrix.

The model parameters are listed in Table 6.

Table 6 : Surface parameters

Magenta words correspond to the names of the python binding parameters

Parameter	Definition	O/ R/C
SURF.Log **ficsurf_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**
SURF.File **ficsurf**	Filename of an user-precomputed surface BRDF/BPDF matrix (full path). *Note : this does not prevent from defining associated parameters that will be useful for analytical calculation of the direct reflection.* By default (and recommended) the reflection matrix is generated by the software. *String (CTE_LENFIC2 characters max)*	**D**
SURF.Alb **rho**	Surface albedo *Float*	**R**
SURF.Type **isurf**	Numéro de type de surface 0 : lambertian surface of albedo SURF.Alb 1 : sunglint (rough sea) 2 : Fresnel reflection (flat sea) 3 : Roujean BRDF 4 : Roujean BRDF + Rondeaux BPDF 5 : Roujean BRDF + Bréon BPDF 6 : Roujean BRDF + Nadal BPDF (not available) 7 : Roujean BRDF+ Maignan BPDF *Integer* Note : the lambertian term SURF.Alb is added to each surface type (it corresponds to the foam reflectance for sunglint simulations).	**R**
If SURF.Type ≠ 0 or 2		
SURF.Dir **dir_surf**	Directory for SURFACE BRDF/BPDF files storage (complete path) *String (CTE_LENDIR characters max)*	**C1**
If SURF.Type ≠ 3 (*for all the models except the Roujean's BRDF)*		
SURF.Ind **surf_ind**	Surface / atmosphere refractive index (air = 1) for the simulation wavelength *Float F5.3*	**C2**

If SURF.Type = 1 (*sunglint)*		
SURF.Glitter.Wind **wind**	Wind velocity at sea surface (m/s) *Float F4.1*	**C3**
If SURF.Type ≥ 3 (*Roujean's BRDF)*		
SURF.Roujean.K0 **SURF.Roujean.K1** **SURF.Roujean.K2** **k0_roujean, k1_roujean, k2_roujean**	Roujean's BRDF model parameters k0, k1 and k2 (in reflectance unit) *Float F5.3*	**C4**
If SURF.Type = 6 (*Nadal's BPDF model)* *OPTION NO LONGER AVAILABLE*		
SURF.Nadal.Alpha **SURF.Nadal.Beta** **alpha_nadal, beta_nadal**	Nadal's model parameter α *Float F6.4* Nadal's model parameter β *Float F4.1*	**C5**
If SURF.Type = 7 (*Maignan's BPDF model)*		
SURF.Maignan.C **coef_c_maignan**	Coefficient C×exp(-NDVI) of the Maignan's BPDF Model *Float F7.3*	**C6**

3.1.5 Parameters for calculating angles

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 the SOS-ABS code. 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 SOS-ABS will generate or use the default filenames.

The conventions for angle definition are explained in section §5.2.3.2, page 68.

Table 7 : Parameters for calculating angles
Magenta words correspond to the names of the python binding parameters

Parameter	Definition	O/D
ANG.Log **ficanglog**	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**

Parameter	Definition	O/D
Angles for radiance computations		
ANG.Rad.NbGauss **nbmu_gauss_lum**	Number of Gauss angles to be used for radiance computations *Integer* Default value (in SOS.h): **CTE_DEFAULT_NBMU_LUM**	**D**
ANG.Rad.UserAngFile **ficangles_user_lum**	Filename (complete path) of a list of user's angles to complete the Gauss angles *String (CTE_LENFIC2 characters max)*	**O**
ANG.Rad.ResFile **ficangles_res_lum**	Filename (without directory tree) of the file created by SOS-ABS, containing the list of angles and maximum orders of series expansions to be used for BRDF/BPDF and radiance computations. *String (CTE_LENFIC2 characters max)* Default value (in SOS.h): **CTE_DEFAULT_FICANGLES_RES_LUM**	**D**
Angles for Mie phase function computations		
ANG.Aer.NbGauss **nbmu_gauss_mie**	Number of Gauss angles to be used for phase matrix computations *Integer* Default value (in SOS.h): **CTE_DEFAULT_NBMU_MIE**	**D**
ANG.Aer.UserAngFile **ficangles_user_mie**	Filename (complete path) of a list of user's angles to complete the ANG.Aer.NbGauss Gauss angles *String (CTE_LENFIC2 characters max)*	**O**
ANG.Aer.ResFile **ficangles_res_mie**	Filename (without directory tree) the file created by SOS-ABS, containing the list of angles and maximum orders of series expansions to be used for phase function computations. *String (CTE_LENFIC2 characters max)* Default value (in SOS.h): **CTE_DEFAULT_FICANGLES_RES_MIE**	**D**

3.1.6 Output parameters

The output parameters defined the choice of provided output data.

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 the “SOS” sub-directory of the working folder (defined by **-SOS_Main.ResRoot**). Therefore, the result filenames are defined without their complete path.

Table 8 : Output parameters

Magenta words correspond to the names of the python binding parameters

Parameter	Definition	R/O
SOS.Log **ficsos_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		
SOS.View **itrphi**	Index of output type: 1 : viewing plane 2 : polar diagram (ascii file) *Integer*	**R**
If SOS.View = 1		
SOS.View.Phi **phios**	Relative azimuth angle (degrees) *Float*	**C1**
If SOS.View = 2		
SOS.View.Dphi **pas_phi**	Azimuth step angle (degrees / integers only) *Integer*	**C1**
Expert parameters		
SOS.IGmax **igmax**	Maximal order of scattering & surface reflexion *Integer* Default value: **100**	**D**
SOS.Ipolar **ipolar**	Index to cut the polarisation (optional) 0 : simulation of SOS-ABS without polarisation If not defined: simulation with polarisation (recommended) *Integer*	**D**
SOS.OutputAlt **zout**	Altitude of the output level (in km): • If not defined: standard output ($L\uparrow_{TOA}$, $L\downarrow_{SURFACE}$) • Z_{out} : upward and downward radiance is given at altitude Z_{out} ($0 \leq Z_{out} \leq$ CTE_TOA_ALT) *Float*	**D**
Output files		
SOS.ResBin **ficsos_res_bin**	Filename of the output binary file from SOS-ABS computations (without directory tree), containing (I,Q,U) in term of Fourier series expansion *String (CTE_LENFIC2 characters max)* Default value (in SOS.h): **CTE_DEFAULT_RESBIN**	**D**

Parameter	Definition	R/O
SOS.ResFileUp	Ascii file name of the output upward field (without directory tree) *String (CTE_LENFIC2 characters max)* Default value (in SOS.h): **CTE_DEFAULT_RESUP**	**D**
SOS.ResFileDown	Ascii file name of the output downward field (without directory tree) *String (CTE_LENFIC2 characters max)* Default value (in SOS.h): **CTE_DEFAULT_RESDOWN**	**D**
SOS.ResFileUp. UserAng	File name of the output upward field restricted to user-defined angles (without directory tree)	**O**
SOS.ResFileDown. UserAng	File name of the output downward field restricted to user-defined angles (without directory tree)	**O**
SOS.Trans **fictrans**	Optional file name (without directory tree) to store transmissions: Direct transmission TOA → surface (BOA). Diffuse transmittance TOA → BOA and BOA → TOA for each viewing angle. If not defined, there is no Transmission file produced. *Note: this option is time consuming.* *The direct transmission is valid for simulation cases that do not take gas absorption into account, or for simulation cases that model the gas absorption using the simplified CKD approach (i.e. when -SOS.AbsModeCKD 2).*	**O**
SOS.Flux **ficflux**	Optional file name (without directory tree) to store TOA and surface fluxes. Downward direct and diffuse fluxes at BOA (normalized by TOA solar flux). Upward diffuse flux at TOA (normalized by TOA solar flux). If not defined, there is no Flux file produced. *Note: The direct downward flux is valid for simulation cases that do not take gas absorption into account, or for simulation cases that model the gas absorption using the simplified CKD approach (-SOS.AbsModeCKD 2).*	**O**

3.1.7 Example of simulation from command lines

The following command file is an example for a radiance simulation at 910 nm, over sea, with a solar zenith angle of 35°, a standard atmospheric pressure, an aerosol optical thickness of 0.3 at 550 nm for the Maritime model of the WMO and a tropical profile to define the water vapour. The Aerosols and molecules profiles of optical thicknesses are defined by an exponential decrease with scale heights: 2 and 8 km, respectively.

The gas absorption is calculated for a 10 cm-1 spectral resolution of CKD coefficients, by using the fine CKD modelling of the absorption / scattering coupling.

The wind velocity is 2 m/s at sea surface. The sea albedo is null for the considered wavelength and the refractive index of the water is 1.34.

The user requires an output of the upward polarized radiance (I,Q,U) field at TOA (default case), in the solar principal plan, for 40 Gauss angles.

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

To perform a simulation, let's run:
$SOS_ABS_ROOT/exe/runSOS-ABS_demo.ksh

```
dirRESULTS=${USER_DIRECTORY}/DEMO_RESULTS
dirMIE=${USER_DIRECTORY }/DATABASE/MIE_AER
dirSURF=${USER_DIRECTORY }/DATABASE/ BRDF_BPDF

$SOS_ABS_ROOT/exe/SOS_ABS_MAIN.exe -SOS_Main.Wa 0.910 \
     -SOS_Main.ResRoot ${dirRESULTS} -SOS_Main.Log SOS_Main_Demo.Log   \
     -ANG.Rad.NbGauss 40 -ANG.Thetas 35. -SOS.View 1 -SOS.View.Phi 0.  \
     -SOS.ResFileUp SOS_Up_Demo.txt                                    \
     -AP.Log Profile_Demo.Log                                          \
     -AP.Psurf 1013  -AP.AerProfile.Type 1 -AP.HR 8.0 -AP.AerHS.HA 2.0 \
     -AP.AbsProfile.Type 1 -AP.SpectralResol 10. -SOS.AbsModeCKD 1     \
     -AER.DirMie ${dirMIE} -AER.Model 1 -AER.WMO.Model 2               \
     -AER.Waref 0.550  -AER.AOTref 0.3                                 \
     -AER.ResFile Aerosols_Demo.txt -AER.Log Aerosols_Demo.Log         \
     -SURF.Dir ${dirSURF}                                              \
     -SURF.Type 1 -SURF.Alb 0.00 -SURF.Ind 1.34 -SURF.Glitter.Wind 2.0
```

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

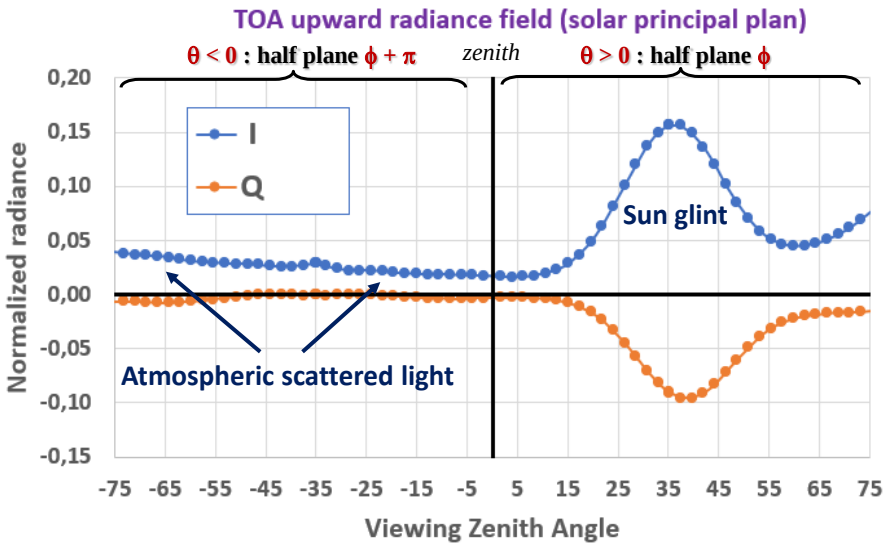

Figure 2 : Illustration of the demo results: normalized radiance at TOA for intensity (I) and polarization (Stokes parameter Q), versus the viewing zenith angle.

3.2 Software constants

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

These constants are taken into account during the compilation phase.

The change of any constant parameter in SOS.h
will only be effective after the re-compilation of the SOS_ABS software.

The SOS.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 aerosol radiative properties.
- Constant values specific to the atmospheric profile definition.
- Constant values specific to computation of surface BRDF/BPDF matrices.
- Constant values specific to the radiative transfer equation calculation, including threshold values for example to check 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.

A modification of the include file SOS.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 9 : List of the constant values in the SOS.h file

Constant	Default value
1) Specific constant values common to all programs	
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**	500
Maximum size of the Keywords for the user's parameters definition **CTE_LENKEYWORD**	30
Length of command system chains	

Constant	Default value
CTE_LENCOM	400
Common constants: Spectral range of application	
Minimal wavelength for radiance calculation (µm)	
CTE_WAMIN	0.364
Maximal wavelength for radiance calculation (µm)	
CTE_WAMAX	4.0
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
2) Specific constants related to the computation of aerosol radiative properties	
Default filename for the aerosol radiative properties definition	
CTE_DEFAULT_FICGRANU	"Aerosols.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.
Minimum value of the Alpha size parameter in MIE's calculus. Must lie between 0,0001 and 10	
CTE_MIE_ALPHAMIN	0.0001D+00
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	0.0001
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_cor_2015_12_16"
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_cor_2015_12_16"
Files containing information on the refractive index of Shettle & Fenn particles (real and imaginary parts) as a function of the wavelength and relative humidity.	

Constant	Default value
CTE_AER_SR_SF	"IRefrac_SR_cor_2015_12_16"
CTE_AER_LR_SF	"IRefrac_LR"
CTE_AER_SU_SF	"IRefrac_SU_cor_2015_12_16"
CTE_AER_LU_SF	"IRefrac_LU_cor_2015_12_16"
CTE_AER_OM_SF	"IRefrac_OM_cor_2015_12_16"
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
Truncation threshold: the phase function truncation is cancelled if the truncation coefficient is lower than this threshold.	
CTE_PH_SEUIL_TRONCA	0.1
Maximal number of modes for an aerosol mixture	
CTE_MAX_NB_MODE_MIXTURE	20
Deviation from 1 tolerated in the summation of optical thickness rates for an aerosol mixture	
CTE_GAP_TOLER_SUM_RATES	0.000001
3) Specific constants related to the calculation of the atmospheric profile	
Standard Pressure (mb)	
CTE_HT_STD_PSURF	1013.
Altitude of the Top of Atmosphere (km)	
CTE_TOA_ALT	120.D+00
Maximum number of atmospheric profile layers	
CTE_OS_NT	600
Optical thickness of an atmospheric layer	
CTE_TCOUCHE	0.005
Optical thickness of the first layer below TOA	
CTE_TOA_FIRST_LAYER_OPT_THICKNESS	0.0002
Step (in km) for the estimate of the altitude of the first layer below TOA	
CTE_DELTA_Z	0.05
Threshold (in km) for the comparison of altitudes while defining the profile of optical thicknesses	
CTE_THRESHOLD_DZ	0.001
Minimum number of atmospheric profile layers	
CTE_OS_NT_MIN	100
Minimum number of molecular sub-layers for a profile with variable positioning of aerosols between 2 altitudes	
CTE_PROFIL_MIN_NBC	3
Definition of the thickness of the transition layer (km)	
CTE_DZTRANSI	0.010
Number of gas to be considered (including line and continuum absorptions): H_2O, CO_2, O_3, N_2O, CO, CH_4, O_2, NO_2	
CTE_NBABS	8
Number of levels of the initial profile of gas	
CTE_ABS_NBLEV	50

Constant	Default value
Number of columns in the files defining the gas absorption profiles	
CTE_ABS_NBCOL	13
Gas to be considered for the simulation of gas absorptions (1 to take the gas into account, 0 otherwise) The absorption of the NO2 is defined only by continuums. The other gases included line and continuum absorptions.	
CTE_ABS_H2O	1
CTE_ABS_CO2	1
CTE_ABS_O3	1
CTE_ABS_N2O	1
CTE_ABS_CO	1
CTE_ABS_CH4	1
CTE_ABS_O2	1
CTE_CONT_NO2	1
Maximum number of wavelengths in the CKD coefficient tables	
CTE_CKD_NWVL_MAX	50
Maximum number of exponentials of the CKD expansion in the tables	
CTE_CKD_NAI_MAX	5
Maximum number of temperatures in the CKD coefficient tables	
CTE_CKD_NT_MAX	9
Maximum number of pressures in the CKD coefficient tables	
CTE_CKD_NP_MAX	31
Maximum number of H2O concentration (for CKD coefficient tables of water vapor)	
CTE_CKD_NC_MAX	12
Maximum wave number covered by the files of CKD coefficient (in cm^{-1})	
CTE_CKD_NUMAX	27500
Minimum wave number covered by the files of CKD coefficient (in cm^{-1})	
CTE_CKD_NUMIN	2500
Number of wavelengths per CKD file (must be the same for all the spectral resolution: 1, 5 ou 10cm^{-1})	
CTE_CKD_NB_NU_PER_FILE	50
Maximal absorption optical thickness (applied for extreme absorptions)	
CTE_TAUABS_MAX	999.
Threshold on absorption optical thickness to optimise the atmospheric profile	
CTE_SEUIL_TAUABS	1.5
4) Specific constants related to the computation of surface reflection matrixes	
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
Threshold value for stopping the expansion in Fourier series of the function (F21 Nadal) / (F21 Fresnel)	

Constant	Default value
CTE_SEUIL_SF_NADAL	0.001
Threshold value for stopping the expansion in Fourier series of Roujean's BRDF **CTE_SEUIL_SF_ROUJEAN**	0.001
Maximum solar zenith angle for computing Roujean's BRDF (degrees). **CTE_TETAS_LIM_ROUJEAN**	60
Maximum viewing zenith angle for computing Roujean's BRDF (degrees). **CTE_TETAV_LIM_ROUJEAN**	60
Threshold value for numerical rounding error tests **CTE_SEUIL_NUM**	1.D-10
5) Specific constants related to the radiative transfer equation calculation	
Default filename for the binary result file of radiance in Fourier series expansion **CTE_DEFAULT_RESBIN**	"SOS_Result.bin"
Default filename for the radiance result file as a function of the zenith angle, for the upward and downward radiance **CTE_DEFAULT_RESUP** **CTE_DEFAULT_RESDOWN**	"SOS_Up.txt" "SOS_Down.txt"
Factor of molecular depolarization in the air **CTE_MDF**	0.0279
Minimum order of the Fourier series expansion **CTE_OS_IBOR**	0
Maximum order of the successive scatterings **CTE_DEFAULT_IGMAX**	100
Threshold to test the convergence of geometric series **CTE_PH_SEUIL_CV_SG**	0.00001
Threshold to stop multiple scattering when the current term (I,Q,U) is low **CTE_PH_SEUIL_VALDIF**	1.0D-50
Threshold to test the stop of cumulative scatterings **CTE_PH_SEUIL_SUMDIF**	0.00001
Threshold to test the stop of Fourier series expansion **CTE_PH_SEUIL_SF**	0.0001
Thresholds to calculate the rotation angles between scattering planes and meridian planes **CTE_SEUIL_Z**	0.0001
Thresholds to transpose the reflexion matrix from the frame tied to the scattering plane to a frame tied to the meridian plane **CTE_SEUIL_X**	**0.00001**
Threshold value under which Q or U is fixed to be null **CTE_THRESHOLD_Q_U_NULL**	1.D-15
Value of the solar disc solid angle (sr) for the mean Earth-Sun distance **CTE_SOLAR_DISC_SOLID_ANGLE**	6.8D-5
Option to remove the binary result -SOS.ResBin if it has already been calculated from a previous simulation (0: it is not removed and the code is stopped, 1: it is automatically removed). Option devoted to expert analysis. **CTE_REMOVE_PREVIOUS_BIN_FILE**	1

Constant	Default value
6) 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**	100
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. **CTE_OS_NBMU_MAX**	80
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 **CTE_OS_NB_MAX**	200
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 **CTE_OS_NS_MAX**	136
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 **CTE_OS_NM_MAX**	336
Default number of angles and maximum orders of series expansions to be used in the case of no definition of angles by the user	
Default number of Gauss' angles (positive values) to be used for the Mie phase function calculations **CTE_DEFAULT_NBMU_MIE**	40
Default number of Gauss' angles (positive values) to be used for the radiance calculations **CTE_DEFAULT_NBMU_LUM**	24
Default value for the limit order of Legendre polynomial and Fourier series expansion to compute radiance:	

Constant	Default value
Usually: CTE_DEFAULT_OS_NB = 2×CTE_DEFAULT_NBMU_MIE **CTE_DEFAULT_OS_NB**	80
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 **CTE_DEFAULT_OS_NS**	48
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 **CTE_DEFAULT_OS_NM**	128
Limitation of the number of angles 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**	20
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**	100
Minimum absolute difference between cos(X) and cos(θ) to assign θ = X **CTE_SEUIL_ECART_MUS**	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**	"SOS_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**	"Aer_UsedAngles.txt"

4. RUNNING A SIMULATION FROM A PYTHON CODE

This chapter describes the input and output parameters to execute a simulation with SOS_ABS code, using the binding python from a python code.

An example is available in the SOS-ABS package: $SOS_ABS_ROOT/**binding/run_sos.py**
(the user can modify the result directory “REP_RES” and the input data directory “REP_DATA” in the example code).

The input and output parameters are explained below:

- The left part before “=sos.sos_proc()”, in blue, is related to the output data.
- The input parameters, in red, are given in the sos.sos_proc function. The value per parameter is supposed to be defined previously. The relation between the name of these input parameters and the parameters for a command line is given in section 3.1.

  Note : parameters “ier” and “trace” are introduced for compliance with the SOS_PROC procedure used from an execution of SOS-ABS by command lines.

  - The parameter “ier” must be set to 0 as initial status of validity of the process. Its value is provided to the calling procedure SOS_ABS_MAIN when using command lines. It is changed to -1 in case of an error occurs during the process.
  - The input parameter “trace” is set as “true” if the user wants a log file for the main process.
- The output parameters, in blue, are defined in Table 10 below.

```
nblum, ind_angout, phi, vza, sca_ang_up, i_up, q_up, u_up, pol_ang_up, pol_rate_up, l_pol_up, \
sca_ang_down, i_down, q_down, u_down, pol_ang_down, pol_rate_down, l_pol_down, \
flux_dir_down, flux_diff_down, flux_tot_down, flux_diff_up, \
coef_tronca = \
   sos.sos_proc(resroot=RESROOT, ficmain_log=FICMAIN_LOG,
                wa_simu=WA_SIMU, nbmu_gauss_lum=NBMU_GAUSS_LUM,
                ficangles_user_lum=FICANGLES_USER_LUM,
                tetas=TETAS, ficangles_res_lum=FICANGLES_RES_LUM,
                nbmu_gauss_mie=NBMU_GAUSS_MIE,
                ficangles_user_mie=FICANGLES_USER_MIE,
                ficangles_res_mie=FICANGLES_RES_MIE,
```

ficanglog=FICANGLOG,
waref_aot=WAREF_AOT, aot_ref=AOT_REF,
itronc_aer=ITRONC_AER,
ficgranu_log=FICGRANU_LOG, ficmie_log=FICMIE_LOG,
dir_mie=DIR_MIE,
ficgranu=FICGRANU, imod_aer=IMOD_AER, rn_wa=RN,
in_wa=IN, rn_waref=RN_WAREF, in_waref=IN_WAREF,
igranu=IGRANU,
lnd_radius_mmd_aer=LND_RADIUS_MMD_AER,
lnd_lnvar_mmd_aer=LND_LNVAR_MMD_AER,
jd_slope_mmd_aer=JD_SLOPE_MMD_AER,
jd_rmin_mmd_aer=JD_RMIN_MMD_AER,
jd_rmax_mmd_aer=JD_RMAX_MMD_AER,
imodele_wmo=IModele_WMO, c_wmo_dl=C_WMO_DL,
c_wmo_ws=C_WMO_WS, c_wmo_oc=C_WMO_OC,
c_wmo_so=C_WMO_SO, imodele_sf=IModele_SF, rh=RH,
mode_param_bilnd=MODE_PARAM_BILND,
user_cv_coarse=USER_CV_COARSE,
user_cv_fine=USER_CV_FINE, rtauct_waref=RTAUct_WAREF,
bmd_cm_mrwa=BMD_CM_MRWA, bmd_cm_miwa=BMD_CM_MIWA,
bmd_cm_mrwaref=BMD_CM_MRWAREF,
bmd_cm_miwaref=BMD_CM_MIWAREF,
bmd_cm_rmodal=BMD_CM_RMODAL,
bmd_cm_var=BMD_CM_VAR, bmd_fm_mrwa=BMD_FM_MRWA,
bmd_fm_miwa=BMD_FM_MIWA,
bmd_fm_mrwaref=BMD_FM_MRWAREF,
bmd_fm_miwaref=BMD_FM_MIWAREF,
bmd_fm_rmodal=BMD_FM_RMODAL,
bmd_fm_var=BMD_FM_VAR,
ficextdata_aer=FICEXTDATA_AER,
ficmixture_aer=FICMIXTURE_AER,
ficuser_aer=FICUSER_AER,
ficprofil_log=FICPROFIL_LOG, tr=TR, hr=HR, ha=HA,
iprofil=IPROFIL, zmin=ZMIN, zmax=ZMAX,
psurf=PSURF, h2o=H2O, o3=O3, co2=CO2, ch4=CH4,
absprofil=ABSPROFIL, ficabsprofil=FICABSPROFIL,
nustep=NUSTEP, isurf=ISURF, dir_surf=DIR_SURF,
ficsurf_log=FICSURF_LOG, surf_ind=SURF_IND,

wind=WIND, k0_roujean=K0_ROUJEAN,
k1_roujean=K1_ROUJEAN, k2_roujean=K2_ROUJEAN,
alpha_nadal=ALPHA_NADAL, beta_nadal=BETA_NADAL,
coef_c_maignan=COEF_C_MAIGNAN, rho=RHO,
ficsurf=FICSURF, ficsos_log=FICSOS_LOG,
ficsos_res_bin=FICSOS_RES_BIN, fictrans=FICTRANS,
ficflux=FICFLUX,
zout=ZOUT, igmax=IGMAX,
ipolar=IPOLAR, itrphi=ITRPHI, phios=PHIOS,
pas_phi=PAS_PHI, imode_ckd_calcul=IMODE_CKD_CALCUL,
ier=IER, trace=TRACE)

Table 10 : General parameters

Parameter	Definition	Type / dimension
Nblum	Number of angles to be considered in the output arrays. nblum ≤ CTE_OS_NBMU_MAX	Integer
ind_angout	Table of values (0 or 1) to define angles in result arrays corresponding to angles defined by the user in the file **ficangles_user_lum** (~ to -ANG.Rad.UserAngFile**)** 1: when the angle is in the user's list 0: otherwise	Array of integers 0 : CTE_OS_NBMU_MAX
Phi	Array of relative azimuth angles for the output radiance field (in degrees). Step of 1 degree.	Array of double precision values 0 : 360
Vza	Array of viewing zenith angles for the output radiance field (in degrees).	Array of double precision values 0 : CTE_OS_NBMU_MAX
sca_ang_up sca_ang_down	Arrays of scattering angles for the upward and downward radiance fields. 2D arrays: • 1st dimension : relative azimuth angles (in degrees). • 2nd dimension : viewing zenith angles (in degrees).	2D Array of double precision values (0 : 360 ; 0 : CTE_OS_NBMU_MAX)

i_up q_up u_up i_down q_down u_down	Arrays of Stokes parameter values I, Q and U for the upward and downward radiance fields (in sr^{-1}). 2D arrays: • 1st dimension : relative azimuth angles (in degrees). • 2nd dimension : viewing zenith angles (in degrees).	2D Array of double precision values (0 : 360 ; 0 : CTE_OS_NBMU_MAX)
pol_ang_up pol_ang_down	Array of polarization angles for the upward and downward radiance field (in degrees).	Array of double precision values 0 : CTE_OS_NBMU_MAX
pol_rate_up pol_rate_down	Array of polarization rate for the upward and downward radiance field (in %).	Array of double precision values 0 : CTE_OS_NBMU_MAX
I_pol_up I_pol_down	Arrays of polarized intensity for the upward and downward radiance fields (in sr^{-1}). 2D arrays: • 1st dimension : relative azimuth angles (in degrees). 2nd dimension : viewing zenith angles (in degrees).	2D Array of double precision values (0 : 360 ; 0 : CTE_OS_NBMU_MAX)
flux_dir_down	Direct transmittance for the sun direction (true atmosphere, no adjustment to the aerosol phase function truncation) As the flux at BOA is normalised by the solar flux at TOA, this value is the direct transmittance from TOA to BOA. *Note: The direct downward flux is valid for simulation cases that do not take gas absorption into account, or for simulation cases that model the gas absorption using the simplified CKD approach (imode_ckd_calcul = 2).*	Double precision
flux_diff_down	Downward diffuse flux at BOA, normalised to the solar flux at TOA.	Double precision
flux_tot_down	Downward total flux at BOA, normalised to the solar flux at TOA.	Double precision
flux_diff_up	Upward diffuse flux at TOA, normalised to the solar flux at TOA.	Double precision
coef_tronca	Truncation coefficient for the aerosol phase function truncation	Double precision

5. INPUT AND OUTPUT FILES

5.1 User input files

The user must provide some input files, depending on the choice of simulation.

5.1.1 User file for angles definition

Specific angles for radiance simulation:

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

It must contain one value per line. No blank line at the end.

Example of a user's angles file defined by -ANG.Rad.UserAngFile
20 25 30 35 40

The calculation of the radiance field will be done for these angles in addition to the Gauss angles. The output files defined by **-SOS.ResFileUp** for the upward radiance (respectively **-SOS.ResFileDown** for the downward radiance) will contain both Gauss and user angles.

By defining an output file with **-SOS.ResFileUp.UserAng** the upward radiance field is only given for the user's angles (respectively **-SOS.ResFileDown.UserAng** for the downward radiance).

Specific angles for aerosol phase function:

The file defined by **-ANG.Aer.UserAngFile** contains a list of scattering angles for which the user wants to get a value of phase function simulations. Only the logfile for aerosol computations (defined by **-AER.Log**). are concerned by this addition of angles to the Gauss angles.

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

Example of a **user's angles file** defined by **-ANG.Mie.UserAngFile**
10 20 30 40 50

Important note:

The filename for a list of user's angles must be changed if the list of angle is modified.

This is because the Mie files and the interface files (BRDF, BPDF matrices) are stored in files whose name includes the file name of the user's angles. They are not recalculated if a Mie file or and interface file with the same name has already been created.

5.1.2 User file for the gas profile definition

The SOS-ABS code is designed to propose the use of predefined gas profiles by setting the parameter **-AP.AbsProfile.Type** from 1 to 7.

But, the users can require the use of their own gas profiles, provided by a formatted file defined by **-AP.AbsProfile.UserFile**, when associated to **-AP.AbsProfile.Type** 0.

The file must contain a fixed number of lines (one line per altitude). The number of altitude levels is defined by CTE_ABS_NBLEV (in the SOS.h file).

For each line, the profile is given by 14 columns (1 + CTE_ABS_NBCOL in SOS.h).

- Column 0 : Level index → *not used*
- Column 1 : Altitude (km)
- Column 2 : Pressure (mbar)
- Column 3 : Temperature (K)
- Column 4 : H_2O concentration (ppmv)
- Column 5 : CO_2 concentration (ppmv)
- Column 6 : O_3 concentration (ppmv)
- Column 7 : N_2O concentration (ppmv)
- Column 8 : CO concentration (ppmv)
- Column 9 : CH_4 concentration (ppmv)
- Column 10 : O_2 concentration (ppmv)
- Column 11 : Density → *data not used currently*
- Column 12 : NO_2 concentration (ppmv)
- Column 13 : SO_2 concentration (ppmv) → *data no more used*

Example of a user's gas profile file defined by -AP.AbsProfile.UserFile

LEVEL ALT(km) P(hPa) T(K) + GASES (ppmv), except column 12: air density

01 0.0 1013.00000 299.7 0.25930E+05 330. 0.28690E-01 0.32000E+00 0.15000E+00 0.17000E+01 0.20900E+06 0.24500E+20 0.23000E-04 0.30000E-03
02 1.0 904.00000 293.7 0.19490E+05 330. 0.31500E-01 0.32000E+00 0.14500E+00 0.17000E+01 0.20900E+06 0.22310E+20 0.23000E-04 0.27400E-03
03 2.0 805.00000 287.7 0.15340E+05 330. 0.33420E-01 0.32000E+00 0.13990E+00 0.17000E+01 0.20900E+06 0.20280E+20 0.23000E-04 0.23600E-03
04 3.0 715.00000 283.7 0.86000E+04 330. 0.35040E-01 0.32000E+00 0.13490E+00 0.17000E+01 0.20900E+06 0.18270E+20 0.23000E-04 0.19000E-03
05 4.0 633.00000 277.0 0.44410E+04 330. 0.35610E-01 0.32000E+00 0.13120E+00 0.17000E+01 0.20900E+06 0.16560E+20 0.23000E-04 0.14600E-03
06 5.0 559.00000 270.3 0.33460E+04 330. 0.37670E-01 0.32000E+00 0.13030E+00 0.17000E+01 0.20900E+06 0.14990E+20 0.23000E-04 0.11800E-03
07 6.0 492.00000 263.6 0.21010E+04 330. 0.39890E-01 0.32000E+00 0.12880E+00 0.17000E+01 0.20900E+06 0.13530E+20 0.23000E-04 0.97100E-04

-
-
-

48 110.0 0.00006 241.6 0.28000E+00 60. 0.50000E-01 0.24430E-03 0.33580E+02 0.95000E-01 0.12000E+06 0.19410E+13 0.23100E-03 0.43200E-04
49 115.0 0.00004 299.7 0.24000E+00 40. 0.50000E-02 0.21200E-03 0.41480E+02 0.60000E-01 0.94000E+05 0.87060E+12 0.17000E-03 0.35800E-06
50 120.0 0.00002 380.0 0.20000E+00 35. 0.50000E-03 0.18510E-03 0.50000E+02 0.30000E-01 0.72500E+05 0.42250E+12 0.17000E-03 0.35800E-06

5.1.3 User file of aerosol radiative properties from an external source

The user can use aerosol radiative properties (phase function, extinction and scattering cross-sections) from an external source by selecting **-AER.Model 4**.

The corresponding file is defined by **-AER.ExtData**.

The format of this file is based on the Oleg Dubovik's tool called DLS [DR5] which provides the primary scattering properties of homogeneous spheroid particles with random orientation. However, the first lines of this format have been revised for SOS-ABS purposes.

This Ascii file 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 cannot exceed the value CTE_MAXNB_ANG_EXT (in SOS.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 SOS-ABS code.

The next lines are not read.

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

```
EXTINCTION_COEF : 0.19941E+00
SCATTERING_COEF : 0.19695E+00
NB_LINES : 163
Angle       F11          -F12/F11    F22/F11     F33/F11
180.00      1.810E-01     0.000E+00  1.000E+00   -1.000E+00
179.14      1.810E-01    -4.686E-07  1.000E+00   -1.000E+00
178.03      1.807E-01    -2.620E-06  1.000E+00   -1.000E+00
176.91      1.803E-01    -7.105E-06  1.000E+00   -1.000E+00
175.79      1.798E-01    -1.498E-05  1.000E+00   -1.000E+00
174.67      1.790E-01    -2.783E-05  1.000E+00   -1.000E+00
173.55      1.781E-01    -4.771E-05  1.000E+00   -1.000E+00
172.43      1.770E-01    -7.729E-05  1.000E+00   -1.000E+00
171.31      1.757E-01    -1.198E-04  1.000E+00   -1.000E+00
170.19      1.743E-01    -1.791E-04  1.000E+00   -9.994E-01
169.06      1.728E-01    -2.595E-04  1.000E+00   -9.988E-01
167.94      1.711E-01    -3.668E-04  1.000E+00   -9.982E-01
166.82      1.692E-01    -5.072E-04  1.000E+00   -9.976E-01
165.70      1.672E-01    -6.872E-04  1.000E+00   -9.970E-01
   •
   •
   •
  7.57      6.896E+00     4.704E-03  1.000E+00    1.000E+00
  6.45      6.954E+00     3.415E-03  1.000E+00    1.000E+00
  5.33      7.003E+00     2.332E-03  1.000E+00    1.000E+00
  4.21      7.043E+00     1.455E-03  1.000E+00    1.000E+00
  3.09      7.073E+00     7.837E-04  1.000E+00    1.000E+00
  1.97      7.095E+00     3.188E-04  1.000E+00    1.000E+00
  0.86      7.106E+00     6.053E-05  1.000E+00    1.000E+00
  0.00      7.109E+00     0.000E+00  1.000E+00    1.000E+00
```

5.1.4 User file for aerosol radiative properties

The user can skip the calculations of the aerosol radiative parameters by providing the optical properties in a file defined by **-AER.UserFile**.

This file can be a result of a previous calculation by SOS-ABS (file defined by **-AER.ResFile**, see details in §0, page 60), or a user made file with the same format.

This functionality can be useful when the user already has Greek coefficients of the aerosol phase functions, the applied truncation coefficient and the single scattering albedo (ratio of scattering and extinction cross sections).

The other values (scattering and extinction cross sections, asymmetry factor) are given for information by SOS-ABS calculations. Their values do not need to be physical correct when the user gives an own aerosol file.

Example of a user's file for aerosol radiative properties defined by -AER.UserFile

```
EXTINCTION CROSS SECTION (mic^2)      :  0.55281E-03
SCATTERING CROSS SECTION (mic^2)      :  0.35911E-03
ASYMMETRY FACTOR (no truncation)      :  0.59091E+00
TRUNCATION COEFFICIENT                :  0.00000
SINGLE SCATTERING ALBEDO (truncation):  0.64961
---------------------------------
PHASE MATRIX COEFFICIENTS FOR K=0 TO  80
ALPHA(K)         BETA11(K)        GAMMA12(K)       ZETA(K)
 0.00000000E+00  0.10000000E+01  0.00000000E+00  0.00000000E+00
 0.00000000E+00  0.17727345E+01  0.00000000E+00  0.00000000E+00
 0.36374787E+01  0.19180056E+01 -0.23829187E+00  0.31245169E+01
 0.20695740E+01  0.15120271E+01 -0.11053269E+00  0.20198381E+01
 0.16113878E+01  0.12125894E+01 -0.89605385E-03  0.14892983E+01
 0.10522072E+01  0.92049984E+00 -0.33483160E-01  0.10488013E+01
 0.89258402E+00  0.73681562E+00  0.27504752E-01  0.83144737E+00
   •
   •
   •
 0.83845465E-02  0.83335960E-02  0.33571593E-05  0.83433842E-02
 0.57265536E-02  0.55903008E-02  0.75284839E-05  0.56814093E-02
 0.28632279E-02  0.28116391E-02  0.53035604E-05  0.28218026E-02
 0.13018169E-03 -0.36410886E-11  0.91978370E-05  0.88671732E-04
```

5.1.5 User file for multi-modes aerosol definition

The user can define an aerosol mixture by combining several particle modes by selecting **-AER.Model 5**. The aerosol parameters are given in a file located by **-AER.DefMixture**.

Example of a user's file defining a mixture of aerosol modes defined by -AER.DefMixture

```
NUMBER OF AEROSOLS MODES: 3

SIZE DISTRIBUTION MODE 1:                                  LND
    MODAL RADIUS (microns):                                0.2
    STANDARD DEVIATION (microns):                          0.1
    REFRACTIVE INDEX at WA_SIMU - Real part:               1.20
    REFRACTIVE INDEX at WA_SIMU - Imaginary part (<0):     -0.0120
    REFRACTIVE INDEX at WA_REF - Real part:                1.4
    REFRACTIVE INDEX at WA_REF - Imaginary part (<0):      -0.014
    PROPORTION TO THE TOTAL AOT at WA_REF:                 0.5

SIZE DISTRIBUTION MODE 2:                                  LND
    MODAL RADIUS (microns):                                0.25
    STANDARD DEVIATION (microns):                          0.15
    REFRACTIVE INDEX at WA_SIMU - Real part:               1.25
    REFRACTIVE INDEX at WA_SIMU - Imaginary part (<0):     -0.0125
    REFRACTIVE INDEX at WA_REF - Real part:                1.45
    REFRACTIVE INDEX at WA_REF - Imaginary part (<0):      -0.0145
    PROPORTION TO THE TOTAL AOT at WA_REF:                 0.1

SIZE DISTRIBUTION MODE 3:                                  JUNGE
    SLOPE:                                                 4.00
    MIN RADIUS (microns):                                  0.01
    MAX RADIUS (microns):                                  50.0
    REFRACTIVE INDEX at WA_SIMU - Real part:               1.4
    REFRACTIVE INDEX at WA_SIMU - Imaginary part (<0):     -0.001
    REFRACTIVE INDEX at WA_REF - Real part:                1.45
    REFRACTIVE INDEX at WA_REF - Imaginary part (<0):      -0.002
    PROPORTION TO THE TOTAL AOT at WA_REF:                 0.4
```

Information included in this file is read successively. Used values must be separated from text by the separator « : ». For each line, the text before the separator is only an indicative text (users are free to write their own text, except to use the separator « : »). The useful values are given after the separator, for each line.

First the file defines the number of used modes. In the SOS.h file, the parameter CTE_MAX_NB_MODE_MIXTURE gives the limit of the number of modes (20 by default), which can be adjusted by the user (requiring a new compilation of the software).

For each block of mode definition, the user defines a model by the keyword « LND » or « JUNGE » in capital letters. For any given model, the code will get its parameters by applying the following sequences:

- If « LND » : modal radius then standard deviation.
- If « JUNGE » : slope, minimal radius then maximal radius.

Then, the user must fill in the value of the refractive index for the wavelength of radiance simulation: real part then imaginary part (negative value).

Afterwards, the user must give the value of the refractive index for the reference wavelength: real part then imaginary part.

> *Note: it is necessary to give the value of the refractive index for the reference wavelength λ_{ref} even if the radiance simulation is made for λ_{ref}.*

Finally, the user must give the relative contribution of each mode to the total aerosol optical thickness for the reference wavelength. The summation of each proportion must equal 1.

5.2 Output files

This chapter describes the content of output files.

5.2.1 File defining the angles used by calculations

The angles used for the calculations are stored in files.

The code generates files containing the information about the angles used to compute respectively phase functions and radiance fields.

Files containing the angles used for calculations	
Param.	User definition : **-ANG.Rad.ResFile**, **-ANG.Aer.ResFile** Default filename in SOS.h, respectively: **CTE_DEFAULT_FICANGLES_RES_LUM**, **CTE_DEFAULT_FICANGLES_RES_MIE**
Location	Directory ***SOS*** in the working folder **(–SOS_Main.ResRoot)**

5.2.1.1 Angles used for radiance calculations

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 provides information on the solar zenith and the corresponding angle index (IMUS). 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)
INTERNAL_IMUS	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 - USER'S ANGLE • • •	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

```
NB_TOTAL_ANGLES :  41
NB_GAUSS_ANGLES :  40
ANGLES_USERFILE
:NO_USER_ANGLES
SOLAR ZENITH ANGLE : 35.000
INTERNAL_IMUS :  16
INTERNAL_OS_NB :  80
INTERNAL_OS_NS :  80
INTERNAL_OS_NM : 160
INDEX   COS_ANGLE            WEIGHT               USER_ANGLE
   1  0.99955382265163D+00 0.11449500031887D-02    0
   2  0.99764986439824D+00 0.26635335895143D-02    0
   3  0.99422754096569D+00 0.41803131246912D-02    0
   4  0.98929130249976D+00 0.56909224514043D-02    0
   5  0.98284857273863D+00 0.71929047681184D-02    0
   6  0.97490914058573D+00 0.86839452692619D-02    0
   7  0.96548508904380D+00 0.10161766041103D-01    0
   •
   •
   •
```

5.2.1.2 Angles used for Mie phase function calculations

The file defined by **-ANG.Aer.Resfile** is used for the Mie computations. The list of angles includes the Gauss angles (and associated weights), as well as the potential angles added by the user (from the file defined by **-ANG.Aer.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.

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

```
NB_TOTAL_ANGLES :  40
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
   •
   •
   •
```

5.2.2 Files defining the radiative properties of aerosols

The SOS-ABS code generates files containing the radiative properties of aerosols.

These files are used to compute the radiance. The format is described below.

Files containing the radiative properties of aerosols	
Param.	User definition : **-AER.ResFile**, Default filename in SOS.h: **CTE_DEFAULT_FICGRANU**
Location	Directory ***SOS*** in the working folder **(–SOS_Main.ResRoot)**
Content	The first eight lines provide comments and formatted data on the extinction and scattering cross-sections (in μm^2), the asymmetry factor, the phase function truncation coefficient, and the single scattering albedo (adjusted to the truncation). The following lines contain the Greek coefficients of the development in 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 polarized phase functions • the **coefficient β(k)** Related to the intensity phase function • the **coefficient γ(k)** Related to the polarized phase functions • the **coefficient ξ(k)** Related to the polarized 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

Example of content of a file -AER.ResFile giving the aerosol radiative properties

```
EXTINCTION CROSS SECTION (mic^2)      :  0.55281E-03
SCATTERING CROSS SECTION (mic^2)      :  0.35911E-03
ASYMMETRY FACTOR (no truncation)      :  0.59091E+00
TRUNCATION COEFFICIENT                :  0.00000
SINGLE SCATTERING ALBEDO (truncation):  0.64961
---------------------------------
PHASE MATRIX COEFFICIENTS FOR K=0 TO  80
ALPHA(K)         BETA11(K)        GAMMA12(K)       ZETA(K)
 0.00000000E+00  0.10000000E+01  0.00000000E+00  0.00000000E+00
 0.00000000E+00  0.17727345E+01  0.00000000E+00  0.00000000E+00
 0.36374787E+01  0.19180056E+01 -0.23829187E+00  0.31245169E+01
 0.20695740E+01  0.15120271E+01 -0.11053269E+00  0.20198381E+01
   •
   •
   •
```

5.2.3 Radiance and degree of polarization for simulation outputs

5.2.3.1 Upward and downward radiance files

The simulation of both radiance and degree of polarization is provided in a devoted file, defined by **-SOS.ResFileUp** (for the upward radiance) or **-SOS.ResFileDown** (for the downward radiance).

Files containing the radiance and degree of polarization	
Param.	User definition : **-SOS.ResFileUp**, **-SOS.ResFileDown** Default filename in SOS.h, respectively: **CTE_DEFAULT_RESUP**, **CTE_DEFAULT_RESDOWN**
Location	Directory ***SOS*** in the working folder **(–SOS_Main.ResRoot)**

By default, the upward radiance is given at TOA and the downward radiance at surface level.
The user can select any altitude in the atmospheric profile with the parameter **-SOS.OutputAlt** (altitude in km). The upward and downward radiance are then provided for this altitude. A linear interpolation is made to estimate the radiance at this altitude from the profile used to simulate the full radiance fields.

If the user defines an output file with the parameter **-SOS.ResFileUp.UserAng** or -**SOS.ResFileDown.UserAng** (respectively for the upward or downward radiance), the result files will contain only the radiance for the user angles (see §5.1.1, page 49).

Results for a given azimuth plan:

If the user wants the radiance fields for a given azimuth plan, the parameter **-SOS.View** must be set to 1, and **-SOS.View.Phi** defines the relative azimuth angle (in degrees) with respect to the direction of the solar light propagation.

Then, the file defined by **-SOS.resFileUp** (respectively **-SOS.resFileDown** for the downward radiance) provides the upwelling radiance field (i.e., the Stokes parameters I,Q,U where I is the radiance) versus the viewing zenith angle, for the given relative azimuth angle **(-SOS.View.Phi**) and for the given altitude **(-SOS.OutputAlt**). The scattering angle, the polarization angle and the degree of polarization (also called polarization rate), as well as the polarized intensity are also provided.

This ascii file is composed of a header which describes in detail the structure of the file and columns data.

Content	Header: 31 lines of information First column: Viewing azimuth angle (in degrees) Second column: Scattering angle (in degrees) Third column: Stokes parameter I (in sr^{-1}) Fourth column: Stokes parameter Q (in sr^{-1}) Fifth column: Stokes parameter U (in sr^{-1}) Sixth column: Polarization angle (in degrees) Seventh column: Degree of polarization (in %) Eighth column: Polarized intensity
Format	Ascii file. **2(2X,F7.2),2X,3(E13.6,2X),2(F7.2,2X),E13.6**

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}**

The unit for I, Q and U is sr^{-1}

Example of a file giving the radiance and degree of polarization:
Filename defined by -SOS.resFileUp in the case -SOS.View 1 and -SOS.View.Phi 0.

```
# UPWARD RADIANCE FIELD VERSUS THE VIEWING ZENITH ANGLE
# (RELATIVE AZIMUTH AND ALTITUDE 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): 180.000
#          for VZA > 0 (sign convention):   0.000
#
# Value of the selected altitude for the output (km) : 300.000
#
# Columns parameters :
#   VZA     :  Viewing Zenith Angle (in degrees)
#   SCA_ANG :  Scattering angle (in degrees)
#   I       :  Stokes parameter I at output altitude z (in sr-1)
#              normalised to the extraterrestrial solar irradiance (PI * L(z) / Esun)
#   Q       :  Stokes parameter Q at output altitude z (in sr-1)
#              normalised to the extraterrestrial solar irradiance
#   U       :  Stokes parameter U at output altitude z (in sr-1)
#              normalised to the extraterrestrial solar irradiance
#   POL_ANG :  Polarization angle (in degrees).  Note: if undefined the value is -999.00
#   POL_RATE:  Degree of polarization (in %)
#   IPOL    :  Polarized intensity at level z (in sr-1)
#              normalised to the extraterrestrial solar irradiance (PI * Lpol(z) / Esun)
#-------------------------------------------------------------------------------------------------
#   VZA     SCA_ANG       I             Q             U         POL_ANG  POL_RATE    IPOL
#(degrees) (degrees)     (sr-1)        (sr-1)        (sr-1)     (degrees)    (%)      (sr-1)
   -88.88   126.12   0.107619E+00  -0.402924E-01  0.000000E+00   -90.00    37.44   0.402924E-01
   -86.65   128.35   0.652788E-01  -0.185523E-01  0.000000E+00   -90.00    28.42   0.185523E-01
   -84.41   130.59   0.537782E-01  -0.125445E-01  0.000000E+00   -90.00    23.33   0.125445E-01
   -82.17   132.83   0.477232E-01  -0.960190E-02  0.000000E+00   -90.00    20.12   0.960190E-02
   -79.94   135.06   0.437624E-01  -0.789604E-02  0.000000E+00   -90.00    18.04   0.789604E-02
   -77.70   137.30   0.409789E-01  -0.685404E-02  0.000000E+00   -90.00    16.73   0.685404E-02
   -75.47   139.53   0.390245E-01  -0.629978E-02  0.000000E+00   -90.00    16.14   0.629978E-02
   -73.23   141.77   0.377092E-01  -0.616402E-02  0.000000E+00   -90.00    16.35   0.616402E-02
   -70.99   144.01   0.368668E-01  -0.646060E-02  0.000000E+00   -90.00    17.52   0.646060E-02
   -68.76   146.24   0.361679E-01  -0.698558E-02  0.000000E+00   -90.00    19.31   0.698558E-02
   -66.52   148.48   0.352511E-01  -0.735644E-02  0.000000E+00   -90.00    20.87   0.735644E-02
    •
    •
```

```
 64.29    80.71   0.473554E-01  -0.182382E-01   0.000000E+00   -90.00    38.51   0.182382E-01
 66.52    78.48   0.510045E-01  -0.174266E-01   0.000000E+00   -90.00    34.17   0.174266E-01
 68.76    76.24   0.558305E-01  -0.169059E-01   0.000000E+00   -90.00    30.28   0.169059E-01
 70.99    74.01   0.617477E-01  -0.165322E-01   0.000000E+00   -90.00    26.77   0.165322E-01
 73.23    71.77   0.687904E-01  -0.161222E-01   0.000000E+00   -90.00    23.44   0.161222E-01
 75.47    69.53   0.769304E-01  -0.157293E-01   0.000000E+00   -90.00    20.45   0.157293E-01
 77.70    67.30   0.863948E-01  -0.153053E-01   0.000000E+00   -90.00    17.72   0.153053E-01
 79.94    65.06   0.972131E-01  -0.150068E-01   0.000000E+00   -90.00    15.44   0.150068E-01
 82.17    62.83   0.109601E+00  -0.150950E-01   0.000000E+00   -90.00    13.77   0.150950E-01
 84.41    60.59   0.123847E+00  -0.162645E-01   0.000000E+00   -90.00    13.13   0.162645E-01
 86.65    58.35   0.141260E+00  -0.205534E-01   0.000000E+00   -90.00    14.55   0.205534E-01
 88.88    56.12   0.178547E+00  -0.407731E-01   0.000000E+00   -90.00    22.84   0.407731E-01
```

Results for a set of azimuth angles (polar angles):

If the user wants the radiance fields for different azimuth plans, the parameter **-SOS.View** must be set to 2, and **-SOS.View.Dphi** defines the step of the relative azimuth angle (in degrees).

Then, the file defined by **-SOS.resFileUp** (respectively **-SOS.resFileDown** for the downward radiance) provides the upwelling radiance field (i.e., the Stokes parameters I,Q,U) versus the viewing zenith and azimuth angles.

This ascii file is composed of a header which describes in detail the structure of the file and columns data.

Content	Header: 26 lines of information First column: Relative Azimuth Angle (in degrees) Second column: Viewing azimuth angle (in degrees) Third column: Scattering angle (in degrees) Fourth column: Stokes parameter I (in sr^{-1}) Fifth column: Stokes parameter Q (in sr^{-1}) Sixth column: Stokes parameter U (in sr^{-1}) Seventh column: Polarization angle (in degrees) Eighth column: Degree of polarization (in %) Nineth column: Polarized intensity
Format	Ascii file. **3(2X,F7.2),1X,3(E13.6,2X),2(1X,F7.2),E13.6**

Example of a file giving the radiance and degree of polarization:
Filename defined by -SOS.resFileUp case -SOS.View 2 and -SOS.View.Dphi 30

```
#UPWARD RADIANCE FIELD VERSUS THE AZIMUTH ANGLE AND VIEWING ZENITH ANGLE
#(ALTITUDE FIXED)
#-------------------------------------------------------------------------------------------------------
# Relative azimuth convention :
#        180° <-> Satellite and Sun in the same half-plan
#          0° <-> Satellite and Sun in opposite half-planes with respect to the zenith directio
#
# Value of the selected altitude for the output (km) : 120.000
#
# Columns parameters :
#   PHI     :  Relative azimuth Angle (in degrees)
#   VZA     :  Viewing Zenith Angle (in degrees)
#   SCA_ANG :  Scattering angle (in degrees)
#   I       :  Stokes parameter I at output altitude z (in sr-1)
#              normalised to the extraterrestrial solar irradiance (PI * L(z) / Esun)
#   Q       :  Stokes parameter Q at output altitude z (in sr-1)
#              normalised to the extraterrestrial solar irradiance
#   U       :  Stokes parameter U at output altitude z (in sr-1)
#              normalised to the extraterrestrial solar irradiance
#   POL_ANG :  Polarization angle (in degrees).  Note: if undefined the value is -999.00
#   POL_RATE:  Degree of polarization (in %)
#   IPOL    :  Polarized intensity at level z (in sr-1)
#              normalised to the extraterrestrial solar irradiance (PI * Lpol(z) / Esun)
#-------------------------------------------------------------------------------------------------------
#   PHI      VZA     SCA_ANG        I              Q              U       POL_ANG  POL_RATE     IPOL
#(degrees) (degrees) (degrees)     (sr-1)         (sr-1)         (sr-1)    (degrees)   (%)       (sr-1)
     0.00     1.71   143.29  0.160129E-01  -0.258388E-02   0.000000E+00    -90.00   16.14 0.258388E-02
     0.00     3.93   141.07  0.157494E-01  -0.244684E-02   0.000000E+00    -90.00   15.54 0.244684E-02
     0.00     6.16   138.84  0.159447E-01  -0.255583E-02   0.000000E+00    -90.00   16.03 0.255583E-02
     0.00     8.39   136.61  0.168233E-01  -0.295572E-02   0.000000E+00    -90.00   17.57 0.295572E-02
     0.00    10.63   134.37  0.187106E-01  -0.371753E-02   0.000000E+00    -90.00   19.87 0.371753E-02
     0.00    12.86   132.14  0.220561E-01  -0.503486E-02   0.000000E+00    -90.00   22.83 0.503486E-02
       •
       •
       •
```

```
    •
  0.00    77.70    67.30  0.834356E-01  -0.138881E-01   0.000000E+00    -90.00   16.65 0.138881E-01
  0.00    79.94    65.06  0.944431E-01  -0.135733E-01   0.000000E+00    -90.00   14.37 0.135733E-01
  0.00    82.17    62.83  0.107448E+00  -0.136143E-01   0.000000E+00    -90.00   12.67 0.136143E-01
  0.00    84.41    60.59  0.123155E+00  -0.146373E-01   0.000000E+00    -90.00   11.89 0.146373E-01
  0.00    86.65    58.35  0.143538E+00  -0.184377E-01   0.000000E+00    -90.00   12.85 0.184377E-01
  0.00    88.88    56.12  0.181348E+00  -0.360266E-01   0.000000E+00    -90.00   19.87 0.360266E-01
 30.00     1.71     0.00  0.160538E-01  -0.138295E-02   0.221495E-02     60.99   16.27 0.261124E-02
 30.00     3.93     0.00  0.157496E-01  -0.137786E-02   0.201986E-02     62.15   15.52 0.244506E-02
 30.00     6.16     0.00  0.157191E-01  -0.146576E-02   0.197984E-02     63.26   15.67 0.246338E-02
 30.00     8.39     0.00  0.160465E-01  -0.166441E-02   0.207637E-02     64.36   16.58 0.266112E-02
 30.00    10.63     0.00  0.168079E-01  -0.200224E-02   0.231018E-02     65.46   18.19 0.305710E-02
 30.00    12.86     0.00  0.180569E-01  -0.249515E-02   0.267073E-02     66.53   20.24 0.365494E-02
    •
    •
    •
 30.00    77.70     0.00  0.698264E-01  -0.114305E-01   0.543351E-02     77.29   18.13 0.126562E-01
 30.00    79.94     0.00  0.789047E-01  -0.115044E-01   0.602243E-02     76.18   16.46 0.129854E-01
 30.00    82.17     0.00  0.896628E-01  -0.118822E-01   0.691355E-02     74.90   15.33 0.137471E-01
 30.00    84.41     0.00  0.102607E+00  -0.131047E-01   0.846133E-02     73.58   15.20 0.155989E-01
 30.00    86.65     0.00  0.119766E+00  -0.167290E-01   0.117953E-01     72.41   17.09 0.204692E-01
 30.00    88.88     0.00  0.154821E+00  -0.322493E-01   0.244949E-01     71.39   26.16 0.404971E-01
 60.00     1.71     0.00  0.161811E-01   0.120428E-02   0.241591E-02     31.75   16.68 0.269942E-02
 60.00     3.93     0.00  0.158914E-01   0.953807E-03   0.233053E-02     33.87   15.85 0.251816E-02
 60.00     6.16     0.00  0.156137E-01   0.748875E-03   0.227401E-02     35.89   15.33 0.239415E-02
 60.00     8.39     0.00  0.153631E-01   0.574975E-03   0.225538E-02     37.85   15.15 0.232751E-02
 60.00    10.63     0.00  0.151389E-01   0.416072E-03   0.226741E-02     39.80   15.23 0.230527E-02
 60.00    12.86     0.00  0.149356E-01   0.262636E-03   0.232230E-02     41.77   15.65 0.233710E-02
    •
    •
    •
```

5.2.3.2 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.

Specific viewing 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 $\pm$ 90° for the horizon.

Figure 3 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:

Area A on Figure 3: Upward direction for a relative azimuth ϕ equals to the value defined by the user (-**SOS.View.Phi**)	$\theta_k > 0$ Propagation toward the zenith: $\theta = 0°$ Propagation toward the horizon: $\theta = 90°$
Area 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: $\theta = 90°$

Area 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: $\theta = -90°$
Area 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: $\theta = -90°$

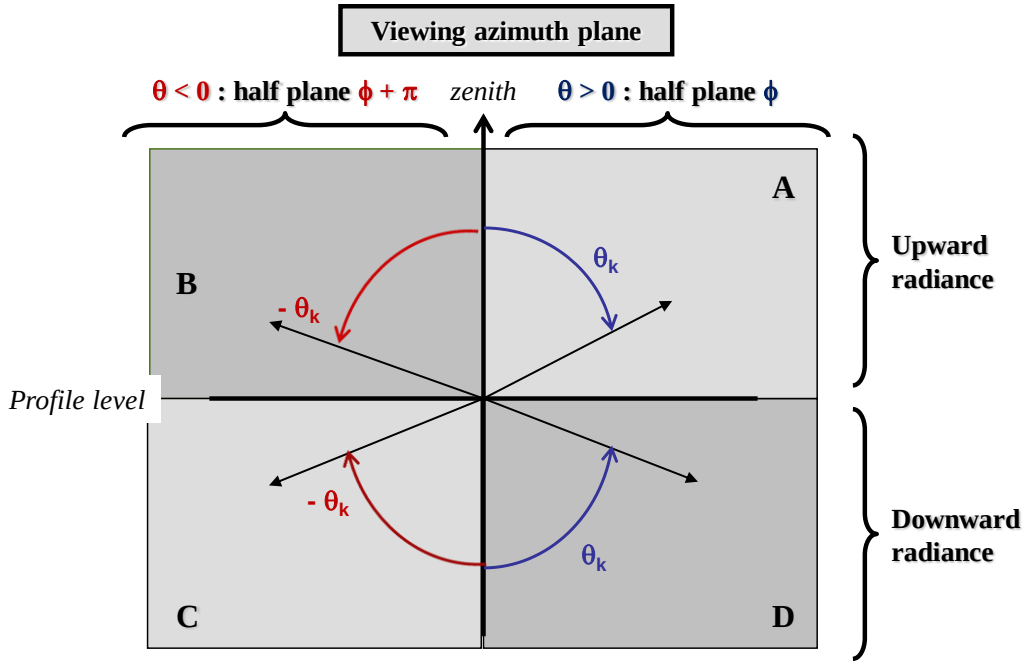

Figure 3 : Convention on zenith angles values for the upwelling and downwelling radiance field. A direction k is illustrated for an upward or downward direction of light propagation. The configuration is shown for each half plane of the relative azimuth, namely ϕ and ϕ+180°.

Figure 4 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. Accordingly, the solar angle used for inner computations is redefined as being 180° - θ_s.

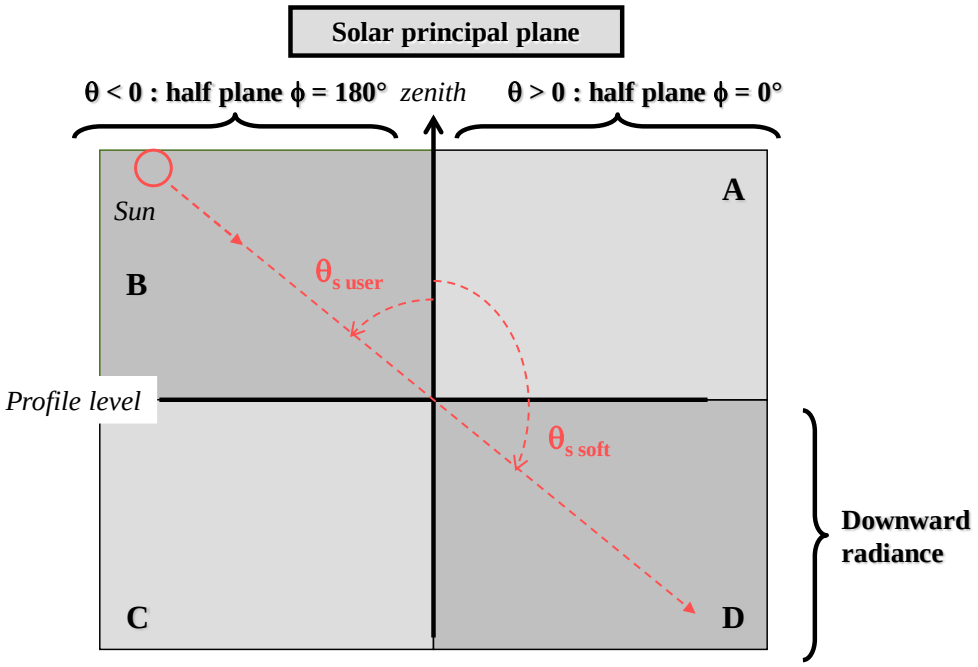

Figure 4 : Location of the Sun in the solar principal plane ($\phi = 180°$). Representation of the solar zenith angle defined by the user and of the solar angle as used by the software with respect to the zenith direction and to the incident direction of the solar beam.

5.2.3.3 Definition of the polarization angle

Let's consider the direction of light propagation $\vec{k}$, the vector $\vec{\ell}$ which is perpendicular to $\vec{k}$ and parallel to the meridian plan (defines by the zenith direction and the direction $\vec{k}$), and the vector $\vec{r}$ such as ($\vec{\ell}$, $\vec{r}$, $\vec{k}$) is a direct orthonormed system.

The angle of polarization is defined on Figure 5 according to the electric field of the polarized light.

As $\begin{cases} Q = E_\ell^2 - E_r^2 \\ U = 2.E_\ell \ .E_r \end{cases}$

one can show: $\begin{cases} \boldsymbol{Q = I_p \times \cos 2\chi} \\ \boldsymbol{U = I_p \times \sin 2\chi} \end{cases}$ (11)

with $I_p = E_\ell^2 + E_r^2$ the intensity of polarization

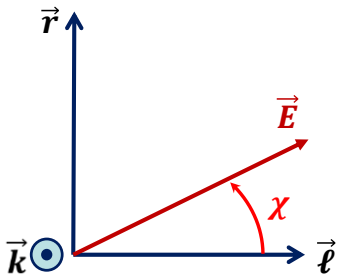

Figure 5 : Polarization angle

The polarization angle is defined in the range: $-\frac{\pi}{2} < \chi \leq \frac{\pi}{2}$

From Q and U values, according to the relation (11) and to the domain of definition of χ, we retrieve the polarization angle by the following algorithm:

If $Q > 0$ then $\chi = \frac{1}{2}\text{atan}(\text{U}/\text{Q})$

If $Q < 0$ then

If $U > 0$ then $\chi = \frac{\pi}{2} + \frac{1}{2}\text{atan}(\text{U}/\text{Q})$

If $U \leq 0$ then $\chi = -\frac{\pi}{2} + \frac{1}{2}\text{atan}(\text{U}/\text{Q})$

If $Q = 0$ then

If $U > 0$ then $\chi = \frac{\pi}{4}$

If $U < 0$ then $\chi = -\frac{\pi}{4}$

If $U = 0$ then χ is undefined

5.2.4 Direct and diffuse transmittance

The user can get the transmittance from the TOA to surface (direct and diffuse parts), and the diffuse transmittance from the surface to TOA. The transmittance is provided for the real atmosphere defined by the user (i.e. not for the equivalent atmosphere adjusted to the aerosol phase function truncation).

The information is given by the file defined by **-SOS.Trans**. It is an optional output, which must be requested only if necessary, because its calculation is time consuming.

Note:
The direct transmission is valid for simulation cases that do not take gas absorption into account, or for simulation cases that model the gas absorption using the simplified CKD approach (i.e. when -SOS.AbsModeCKD 2).

File containing the values of transmittance	
Param.	User definition : **-SOS.Trans** Optional.
Location	Directory ***SOS*** in the working folder **(–SOS_Main.ResRoot)**
Content	The file reminds the Solar Zenith Angle (SZA). It gives the direct and diffuse transmittance from TOA to ground for the SZA. It gives also the upward diffuse transmittance from surface to TOA for the different viewing angles.
Format	Ascii file.

Example of a file giving the transmission profile:
Filename defined by -SOS.Trans

```
Solar Zenith Angle :  35.000
Direct transmission TOA -> surface :   0.6176

 Diffuse transmittance : TOA -> surface
    thetas = 35.000   td(thetas) =  0.1711

 Diffuse transmittance : surface -> TOA
    thetav =  1.712   td(thetav) =  0.1532
    thetav =  3.929   td(thetav) =  0.1534
    thetav =  6.159   td(thetav) =  0.1537
    thetav =  8.393   td(thetav) =  0.1541
    thetav = 10.627   td(thetav) =  0.1547
    thetav = 12.862   td(thetav) =  0.1554
    thetav = 15.097   td(thetav) =  0.1563
   •
   •
   •
```

5.2.5 Downward flux at BOA and upward flux at TOA

The user can obtain the calculated flux at BOA (direct and diffuse downward fluxes) and the upward diffuse flux at TOA, by defining the result file with **-SOS.Flux** (optional request).

Let's note all the values of flux are normalised to the solar irradiance at TOA. This means that the direct downward flux at BOA is equal to the direct transmittance.

Note: The direct downward flux is valid for simulation cases that do not take gas absorption into account, or for simulation cases that model the gas absorption using the simplified CKD approach (i.e. when -SOS.AbsModeCKD 2).

BOA and TOA flux	
Param.	User definition : **-SOS.Flux** Optional.
Location	Directory ***SOS*** in the working folder **(–SOS_Main.ResRoot)**
Content	The file gives the Solar Zenith Angle (SZA). It gives the direct and diffuse downward flux at BOA. It gives also the upward diffuse flux at TOA. The values of flux are normalised to the solar irradiance at TOA. The atmospheric profile is reminded : Molecular Optical Thickness (MOT), Aerosol Optical Thickness (AOT), Gas Optical Thickness (GOT),
Format	Ascii file.

Example of file giving the downward flux at BOA and upward flux at TOA:
Filename defined by -SOS.Flux

```
Solar Zenith Angle :  40.000

 Downward fluxes at BOA (normalized by TOA solar flux)
   - Downward direct flux at BOA :    0.1562
   - Downward diffuse flux at BOA:    0.0582
   ==> Downward total flux at BOA:    0.2144

 Upward diffuse flux at TOA (normalized by TOA solar flux):  2.1411568E-002

 According to the following profile
 Z(km)     MOT      AOT      GOT      TOTAL
 120.00    0.0000   0.0000 -0.0000   0.0000
     •        •        •        •        •
     •        •        •        •        •
     •        •        •        •        •
   2.00    0.0066   0.1406   0.6438   0.7910
   1.00    0.0075   0.2317   0.8353   1.0746
   0.00    0.0085   0.3821   1.0317   1.4222
```

5.2.7 Log files

The different logfiles are listed in Table 11.

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

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

Table 11 : List of logfiles

Logfile parameter	Content
-SOS_Main.Log	The main logfile gives information on the different routine executions (input/output parameters, warnings, error cases, …)
-ANG.Log	This logfile gives information about the angle computations: Gauss angles used for the phase functions and radiance calculations, solar zenith angle, user's angles.
-AP.Log	This logfile gives information about the atmospheric profile computation.
-AER.Log	This logfile gives information about the computation of the radiative properties 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 matrix phase functions (polarized form) versus the size parameter from Mie calculations.
-SURF.Log	This logfile gives information about the calculation of surface BRDF/BPDF matrices: Fresnel matrices, probability function of the wave orientation, …
-SOS.Log	This logfile gives information about the successive orders of scattering computation (core of the radiative transfer code).