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Successive Order of Scattering radiative transfer code (version 5.0)

User Guide

Prepared by **Bruno LAFRANCE** (CS SI)

CS SI

Parc de la Plaine

5 Rue Brindejone des Moulinais

BP 15 872

31506 Toulouse Cedex 5 - France

mail: bruno.lafrance@c-s.fr

tel: (33) 5 61 17 63 93

Software distribution by **Olivier HAGOLLE** (CNES / CESBIO)

CNES (DCT/SI/MO) and CESBIO

BPI 811

18 avenue Edouard Belin

31401 Toulouse Cedex 9- France

mail: olivier.hagolle@cnes.fr

tel : (33) 5 61 28 21 35

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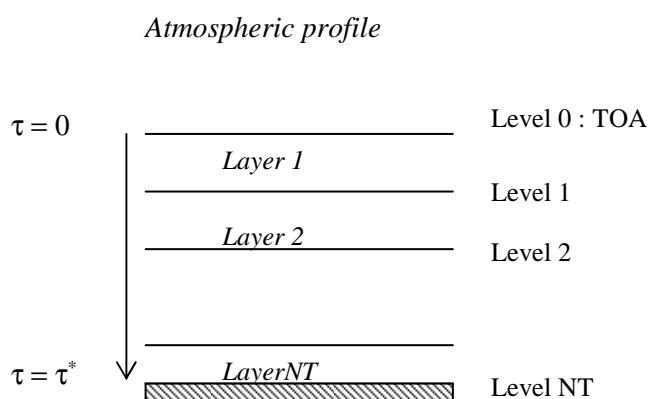
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I- Introduction

The *Successive Order of Scattering* code simulates the scattered and polarized radiance of the system {surface – atmosphere}, under a clear sky and without gaseous absorption.

The concentration profile of particles (aerosols and molecules) is modelled through the division of the atmosphere in layers of optical thickness. For each level, considering the particle mixture, a phase matrix characterizes the scattering properties of the layer right above.



Light propagation through the atmosphere is described by the Equation of Radiative Transfer (ETR). At each level, the SOS code starts by computing the radiance field caused by the single-scattering of the direct solar beam (the solar irradiance is set equal to π in order to compute normalized radiance values). From these first radiation fields, one may derive the global field of single-scattering: by integrating the ETR for the upward field (considering the surface reflection of the direct solar beam) or for the downward field, the SOS code computes iteratively (layer after layer) the single scattering radiance emerging at TOA or illuminating the ground. The polarized radiance is computed as well.

This radiance field of order 1 induces the 2nd surface reflection and the source function of the 2nd scattering at each level of the atmospheric profile. The global radiation field of order 2 is then obtained by the same type of solution as for the single-scattering. By computing iteratively the successive terms of interaction and by adding them, we obtain the global field of radiance for each layer.

The complexity of the method lies on the expansion into Fourier series of the azimuth in order to separate zenith-dependent terms from azimuth-dependent terms in the expression of the radiance. This mathematical formalism is used to speed up the processing by a significant amount.

The complexity of the method lies on the use of Fourier series expansion in order to separate zenith-dependent terms from azimuth-dependent terms in the expression of the radiance. This mathematical formalism is used to speed up the processing by a significant amount.

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The SOS code was first implemented by M. Deuzé during his PhD studies, which were dealing with the polarization of light by scattering media [Laboratoire d’Optique Atmosphérique, 1974, DR4]. The code was then extended to enable simulation of the sunglint reflection by the sea [1989, DR5].

The current version of the SOS code integrates the initial functions with new and improved methods of simulation:

- The aerosol data base has been widened : it is now possible to simulate mono-modal particle size distribution model (log or Junge function) as well as more complex models such as bimodal distributions [DR6] or predefined models from WMO [DR19] and Shettle & Fenn [DR15] (continental, urban, maritime or coastal models which consider relative air humidity). It is also possible to import phase functions from an external source which can be used to simulate scattering effects of non-spherical aerosols (with a random orientation). The position of the aerosol layer may be modified in the atmospheric profile definition.
- The use of new surface conditions is made possible: reflection model by Roujean [DR14], reflection model with polarisation by Rondeaux [DR13] for vegetation or by Bréon [DR2] for bare ground, semi-empirical model by Nadal [DR12].

The software code has gone through a refactoring phase, which included corrections of anomalies, adding of comments, reorganisation and optimization. The computation time has significantly decreased. The use of the software has been simplified: processing parameters are defined by “-Keyword *Value*”; the angles for Gauss quadrature and the associated values for limit orders of expansion are defined by the code.

This document is the user manual of the **version 5.0** of the **Successive Order of Scattering** code.

It contains the description of the installation procedure and operating modes.

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II- Installation

II-1 Software and hardware environment

The SOS software runs on a :

- SUN machine with SOLARIS operating system,
- PC with RedHat LINUX.

using a **Fortran** compiler (g77 or f77).

Note: The application outputs binary files (Mie calculations and surface reflection matrices) which formats are not compatible between SUN and PC architectures (data are recorded with different endianness : Most Significant Bit First against Least Significant Bit First).

II-2 SOS Arborescence

The SOS arborescence must first be copied on the user account.

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

-src : contains the sources

- SOS_ANGLES.F : manages angles and expansion orders.
- SOS_AEROSOLS.F : computes aerosol radiative parameters.
- SOS_MIE.F : generates MIE files
- SOS_PROFIL.F : defines the atmospheric profiles
- SOS_SURFACE.F : generates surface BRDF / BPDF files
- SOS_GLITTER.F : computes reflection matrices for sun glint
- SOS_ROUJEAN.F : computes Roujean's BRDF matrices
- SOS_RONDEAUX_BREON.F : generates BPDF matrices from Rondeaux or Bréon models
- SOS_NADAL.F : generates BPDF matrices from Nadal model.
- SOS_NOM_FIC_SURFACE.F : manages file names of surface reflection matrices
- SOS.F : main program for successive scattering computations.
- SOS_OS.F : computes the scattered and polarised radiance field (I, Q, U) for a diffuse atmosphere.
- SOS_TRPHI.F : outputs result files for Stokes parameters I, Q, U.

-obj : folder for compiled files.

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-exe : contains all executables and a KSH launch script

5 executables :

SOS_ANGLES.exe generates the files for the angles

SOS_AEROSOLS.exe generates the aerosol files,

SOS_PROFIL.exe generates the atmospheric profiles

SOS_SURFACE.exe generates the surface reflection matrices

SOS.exe computes the successive order of scattering.

2 ksh files (KornShell) :

runOS.ksh allows to select simulation parameters and feeds the main script **main_SOS.ksh** with arguments,

main_SOS.ksh supervises the workflow and calls the different executables.

1 text file:

config.txt is a copy of the file « **SOS.h** » (cf. §III-3). It contains the values of all constant parameters which were used for the compilation.

-inc : contains the file « **SOS.h** » which lists all constant parameters (cf. §III-3). All programs share this file. It specifies the size of 2D-arrays, names of data files issued from WMO and Shettle & Fenn aerosol models, as well as required thresholds.

-gen : contains Makefiles used for compilation and link.

-fic : contains data files required for the processing :

Aerosol data files from WMO and Shettle & Fenn models: *DataWMO, DataSF, IRefrac_LR, IRefrac_LU, IRefrac_OM, IRefrac_SR, IRefrac_SU.*

-doc : contains 5 text files :

Install.txt : installation from the SOS code.

Fichier.txt : description of file contents used by the SOS code.

Manuel.txt : execution of SOS code.

SOS-MU-001-II-E3-R0 : user guide (French version) in Microsoft Word format (.doc) and PDF format (.pdf).

SOS-UG-001-II-E1-R0: user guide (English version) in Microsoft Word format (.doc) and PDF format (.pdf).

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II-3 Compiling

- a) As a precaution, suppress all object files .o (rm *.o) in the directory *obj*.
- b) assign the environment variable RACINE to the SOS main folder's path.

Example : export RACINE=/users/username/SOS.

Type "ls \$RACINE" to display all sub-directories described in section II-2.

It is recommended to define the variable \$RACINE in a « .profile » or « .kshrc » file of the user account so as to avoid redefining it every time.

- c) change directory to gen (cd \$RACINE/gen).
- d) run the makefile :

make -f Makefile.xxx

with xxx=g77 if the compiler g77 is available,

avec xxx=f77 if the compiler f77 is available.

Upon completion, one can find :

- In \$RACINE/obj : object files output by the compiler,
- In \$RACINE/exe :
5 executables SOS.exe, SOS_AEROSOLS.exe, SOS_ANGLES.exe, SOS_PROFIL.exe and SOS_SURFACE.exe in addition to the KSH scripts.

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III- Operating mode

This chapter describes the procedure required in order to execute a simulation.

The processing parameters are divided in two sets :

- parameters specific to the simulation, specified in **runOS.ksh**,
- dimensioning parameters and threshold values defined in the include file **SOS.h**.

The parameters are interactively entered by the user when calling the main script **main_SOS.ksh**. It is also possible to define the parameters directly in the script **runOS.ksh** (under \$RACINE/exe) which sets the required environment variables and executes main_SOS.ksh. The script **runOS.ksh** specifies all simulation parameters : physical parameters describing surface properties (albedo, BRDF, BPDF) and atmosphere content (molecules, aerosols), as well as the solar angle. **runOS.ksh** also allows to specify the type of desired output (viewing for a given plan of azimuth or global field of view, profile level, maximum order of interactions, switching off polarisation) as well as required angles (number of Gauss angles for spatial integrations, and list of user-defined angles). The user may also define the names of the output files, log files, and the arborescence for storing Mie and BRDF or BPDF files.

The **include file SOS.h** (under \$RACINE/inc) contains all simulation constant parameters. It defines all dimensioning parameters which values are taken into account at compilation time.

***Any change made to a constant parameter must be followed
by software recompilation to become effective.***

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 SOS_AEROSOLS methods.
- Constant values specific to atmospheric profile definition.
- Constant values specific to computation of surface reflection matrices.
- Constant values specific to SOS methods, including threshold values in particular for testing whether the end of the processing has been reached.
- Constant values specific to angle definition and orders for the Fourier series and Legendre polynomials expansions.

Modification of the include file SOS.h is rarely necessary. Any change to its content requires a detailed knowledge of the software.

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III-1 Defining the environment variables

All paths to executables, input and output files are defined by the environment variables which are set by **runOS.ksh**.

runOS.ksh requires 3 environment variables :

- **\$SOS_RACINE** is set to the **\$RACINE** variable which itself points to the root directory of the software (refer to II-3).
- **\$SOS_RESULT** specifies the output directory.
- **\$SOS_RACINE_FIC** specifies the directory for predefined aerosol data files (WMO and Shettle&Fenn models).

Environment variables		runOS.ksh
<i>Nom</i>	<i>Description</i>	
SOS_RACINE	Path to the SOS arborescence	
SOS_RESULT	Path to the output files	
SOS_RACINE_FIC	Path to predefined aerosols files (WMO and Shettle & Fenn models)	

III-2 Defining simulation parameters

There are 5 sets of parameters:

- Parameters for required angles.
- Base parameters for radiation field.
- Parameters for surface conditions.
- Parameters for the atmospheric profile (optical thickness).
- Parameters for aerosols.

These parameters are defined by « **-Keyword Value** » during the call to main_SOS.ksh.

Chapter III-2.1 lists all simulation parameters.

Chapter III-2.2(p. 25) defines parameters for angular conditions.

Chapter III-2.3 (p. 28) defines parameters relative to surface conditions.

Chapter III-2.4 (p. 33) defines the atmospheric parameters.

Chapter III-2.5 (p. 42) defines the output type.

Chapter III-2.6 (p. 46) defines available output files

Finally, Chapter III-2.7 (p. 47) illustrates a simulation.

III-2.1 Parameter list

The following sketches indicate the input parameters (Keyword) to main_SOS.ksh.
 Table 1 further describes all parameters.

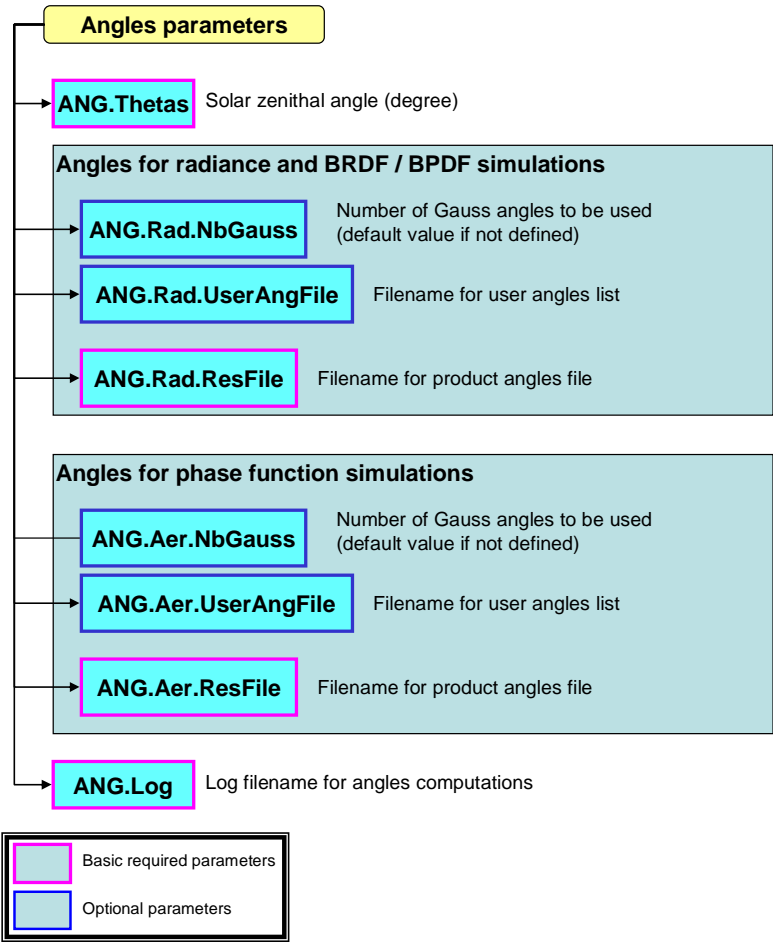


Figure 1 : main_SOS.ksh parameters for angle definition

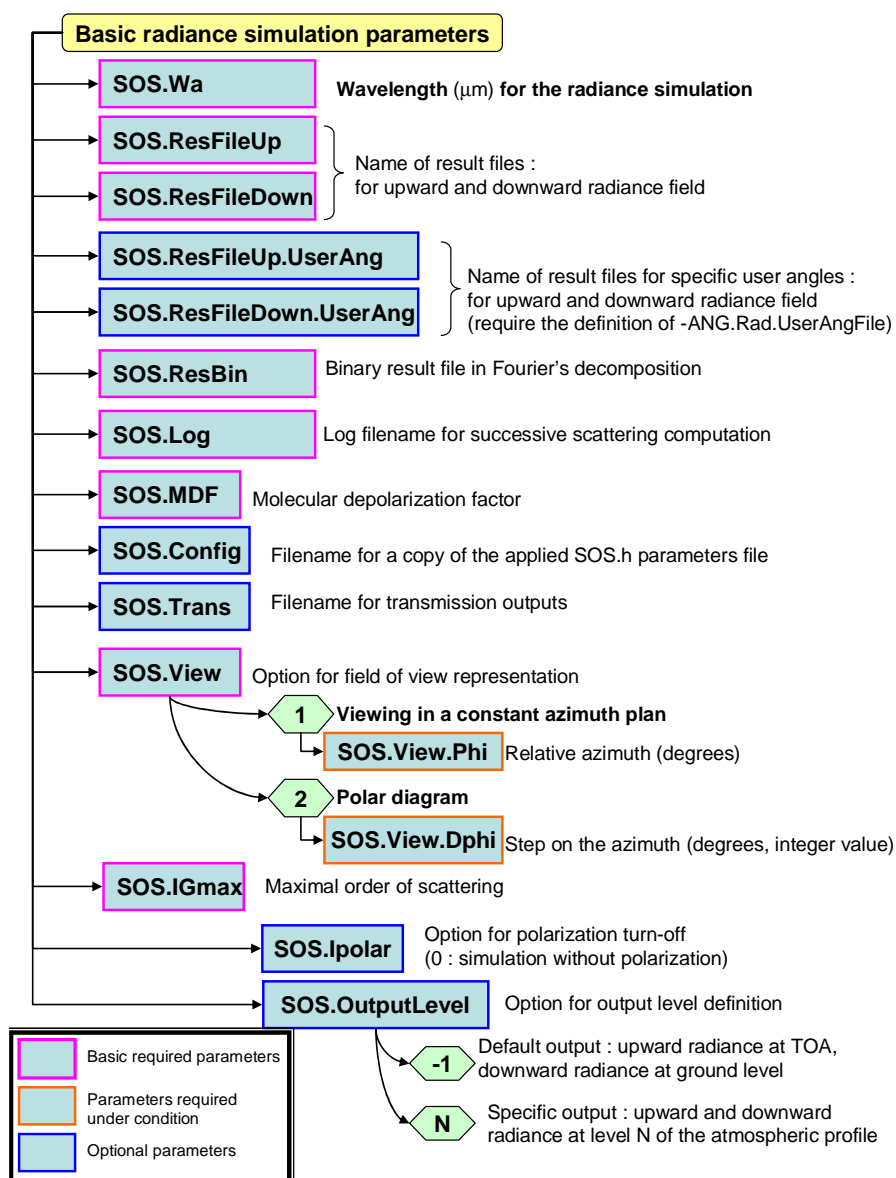


Figure 2 : main_SOS.ksh base parameters for radiation field simulation

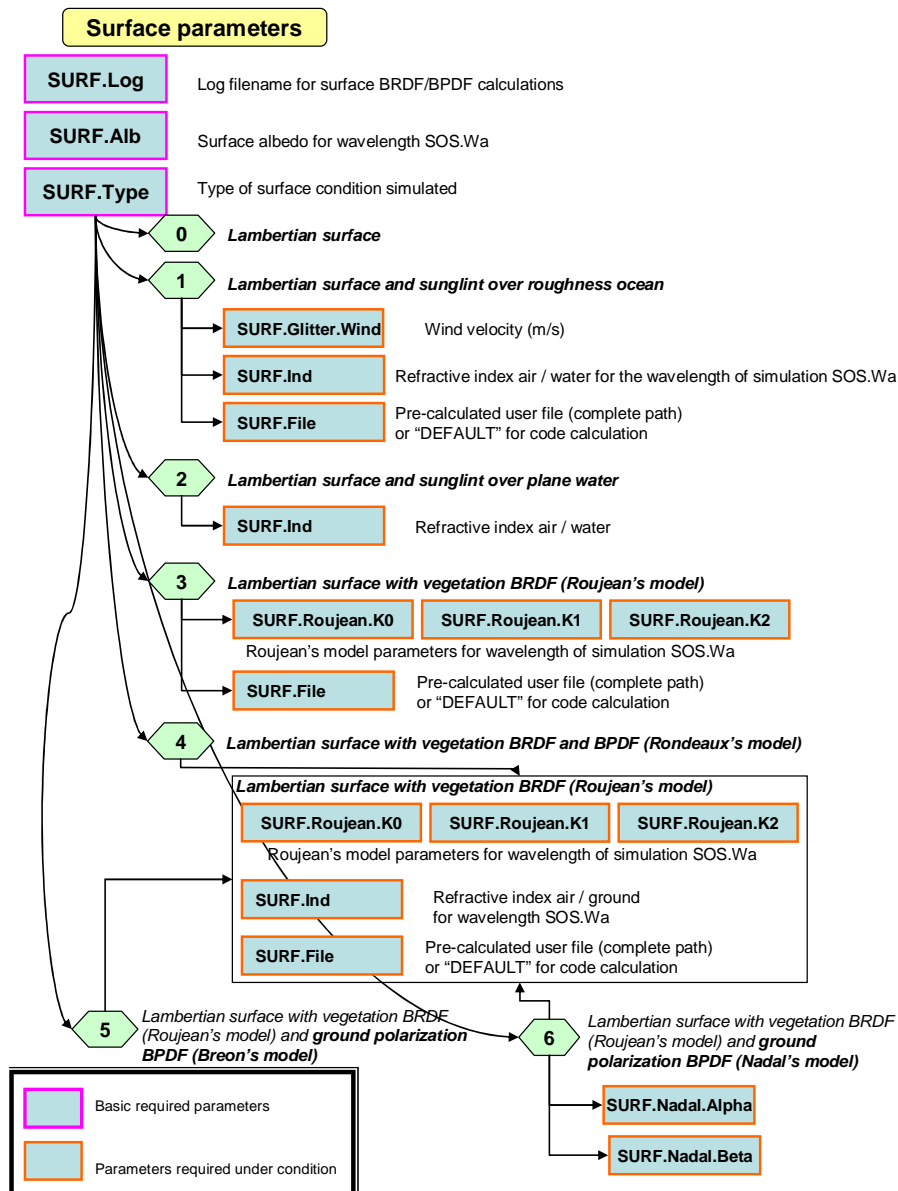


Figure 3 : main_SOS.ksh parameters for surface conditions

Atmospheric Profile

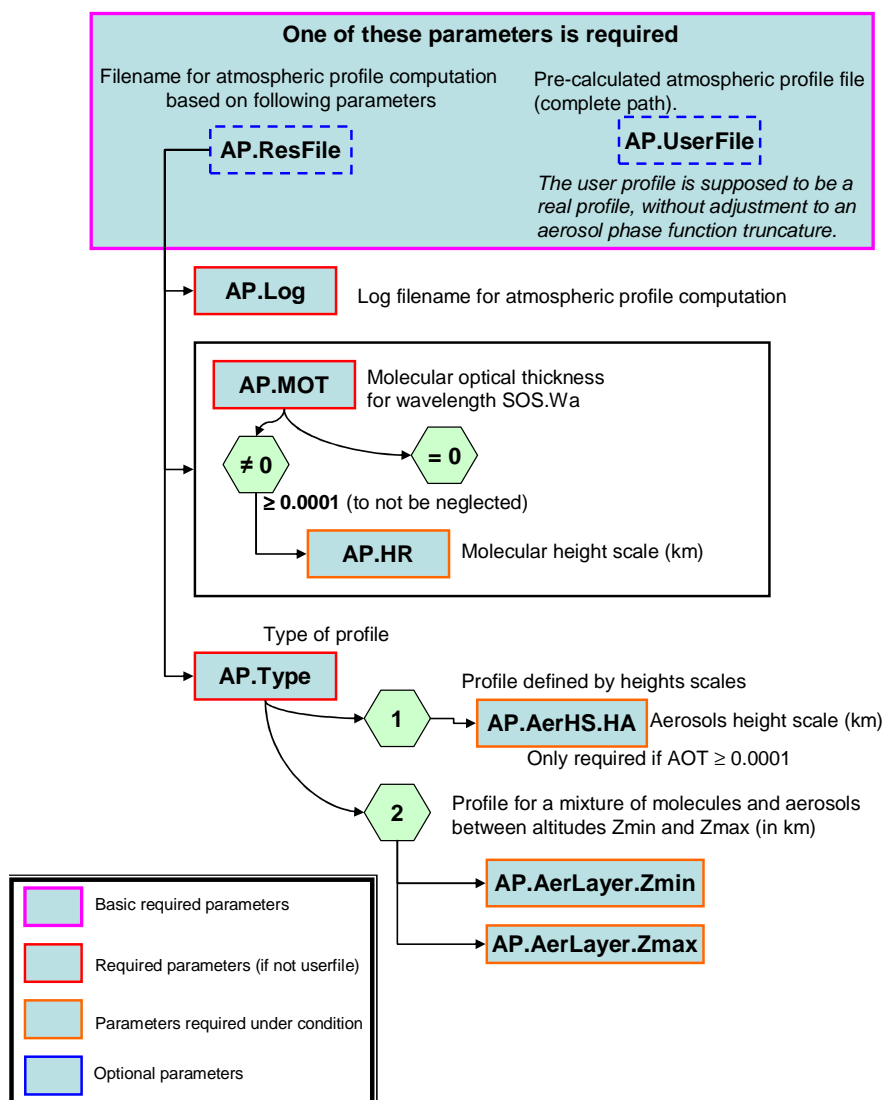


Figure 4 : main_SOS.ksh parameters for atmospheric profiles

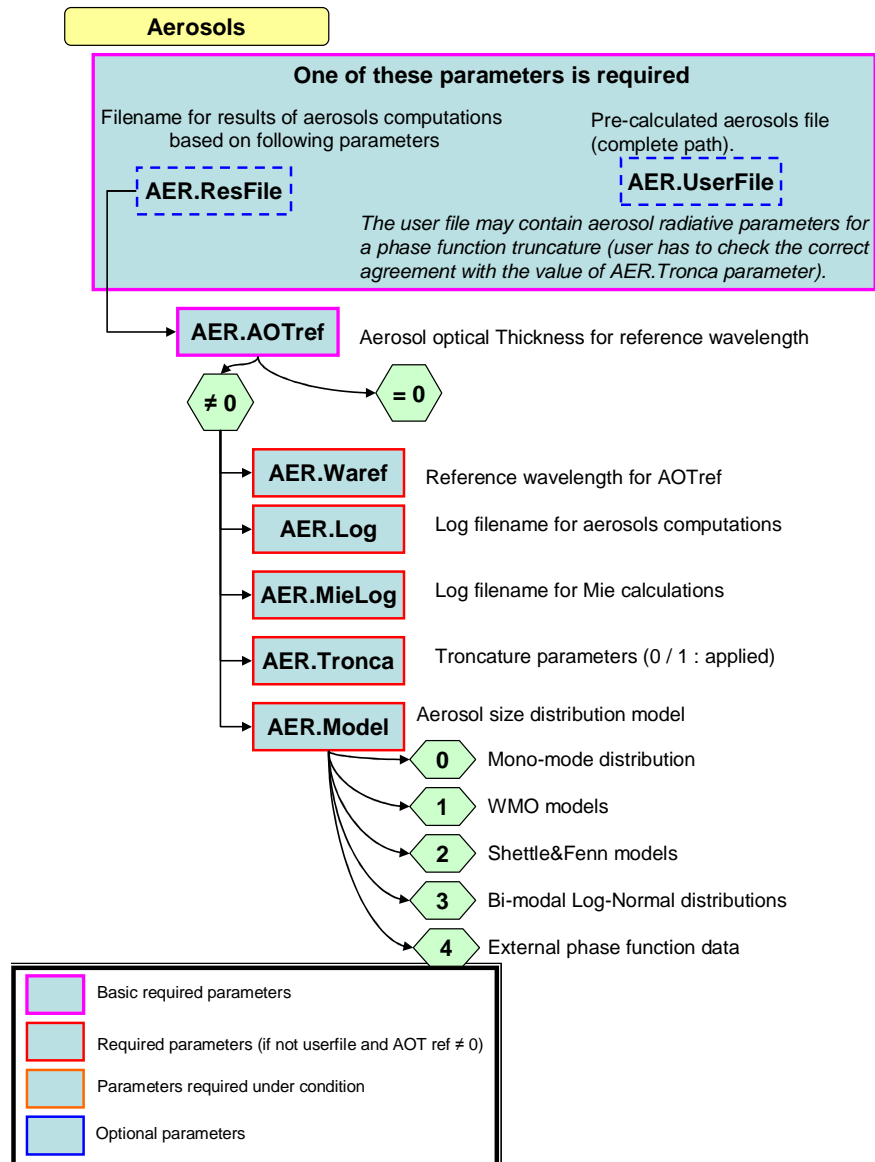


Figure 5 : main_SOS.ksh parameters for aerosols (1/2)

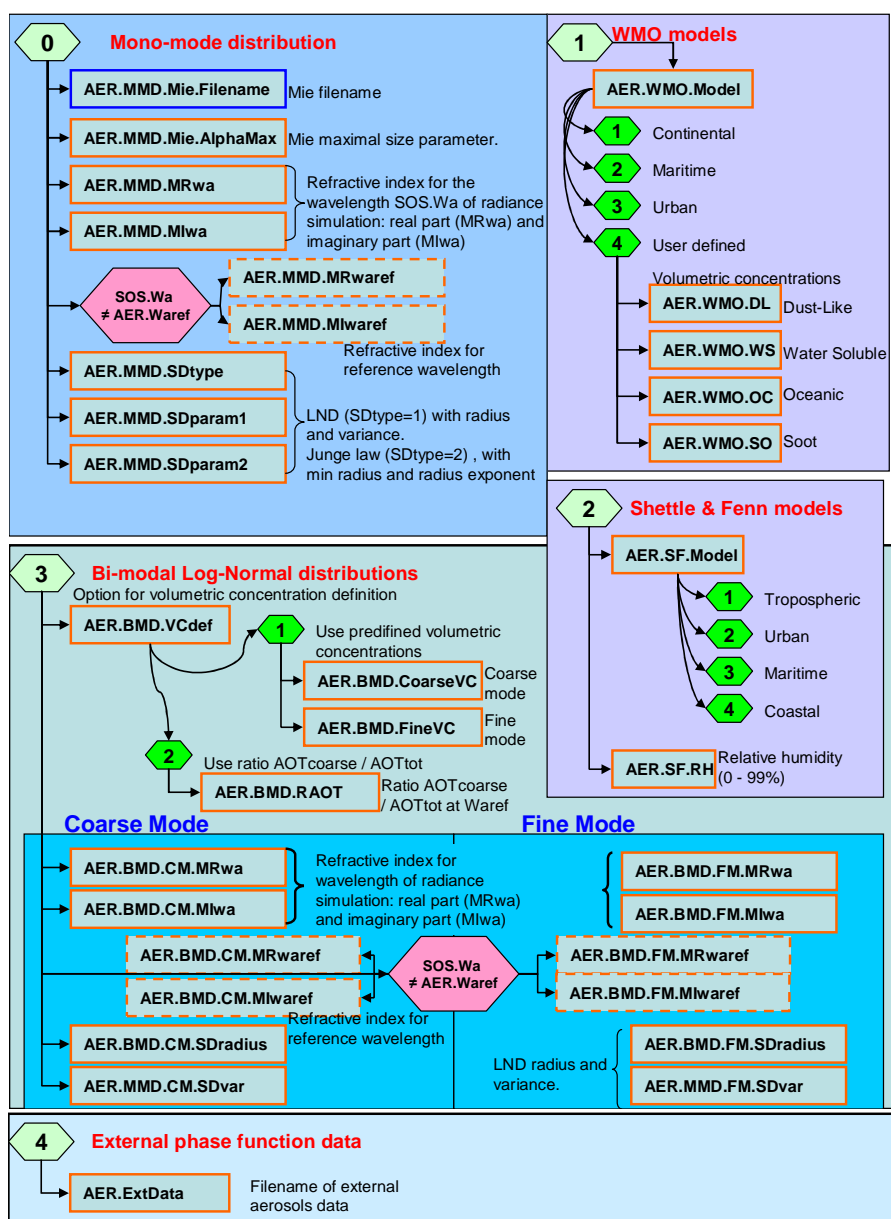
AER.Model Aerosol size distribution model

Figure 6 : main_SOS.ksh parameters for aerosols (detailed options) (2/2)

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Tableau 1 : Simulation parameters

Simulation parameters :	
Description of inputs, outputs, physical parameters, and processing options	
<i>Directories for surface reflection files, Mie files, Log files and output files.</i>	
dirSUNGLINT	Directory for sun glint model reflection files
dirROUJ	Directory for Roujean model reflection files
dirRH	Directory for Rondeaux – Herman model reflection files
dirBREON	Directory for Bréon model reflection files
dirNADAL	Directory for Nadal model reflection files
dirMIE	Directory for Mie files
dirLOG	Directory for log files
dirRESULTS	Directory for output files
<i>SOLAR INCIDENCE PARAMETERS AND DEFINITION OF ANGLES</i>	
ANG.Thetas	Solar zenith angle in degrees ($0 < \text{thetas} < 90^\circ$)
ANG.Rad.NbGauss	Number of Gauss angles for radiance and BRDF/BPDF simulations
ANG.Rad.UserAngFile	File name of additional user-defined angles for radiance computations.
ANG.Rad.ResFile	Output file name of angles and maximum orders of series expansion to be used for radiance computations.
ANG.Aer.NbGauss	Number of Gauss angles for phase functions
ANG.Aer.UserAngFile	File name of additional user-defined angles for phase functions.
ANG.Aer.ResFile	Output file name of angles and maximum orders of series expansion to be used for phase functions.
ANG.Log	Log filename for the ANGLES function <i>Enter 0 for no log file</i>
<i>WAVELENGTH FOR RADIANCE SIMULATION</i>	
SOS.Wa	Wavelength for radiance simulation (μm)
<i>ATMOSPHERIC PROFILE PARAMETERS</i>	
AP.Log	Log file name of the executable named PROFIL <i>Enter 0 for no log file</i>
AP.ResFile	PROFIL file name: <i>Used if no User file</i> Note : File overwritten by each run
AP.userFile	File name for user-precomputed atmospheric profile (full path) Note :the user profile is assumed to be a real profile which has not undergone adjustment with respect to the truncation of the aerosol phase function.
<i>Molecules</i>	
AP.MOT	Rayleigh optical thickness
<i>If AP.MOT ≥ 0.0001</i>	
AP.HR	Height scale of the molecular profile (km)

AEROSOLS PARAMETERS	
AER.MieLog	Log filename of Mie calculations <i>Enter 0 for no log file</i>
AER.Log	Log filename of the AEROSOLS executable <i>Enter 0 for no log file</i>
AER.ResFile	Default file name for AEROSOLS output File overwritten by each run
AER.UserFile	File name for user-precomputed Aerosols radiative properties (full path). <i>Note : The file Aerosols includes the information relative to truncation if has occurred. It can only be used if processing is performed on the same wavelength as for the simulation (reference wavelength identical to the wavelength for simulation of the radiation field).</i>
AER.Waref	Reference wavelength (μm) for simulation of aerosol radiative properties
AER.AOTref	Aerosol optical thickness for the reference wavelength
AER.Tronca	Phase function truncation 0 : no 1 : yes
<i>Aerosols : size distribution model</i>	
AER.Model	Type of aerosol models 0 : mono-modal 1 : WMO multi-modal 2 : Shettle & Fenn bi-modal 3 : Log-Normal bi-modal 4 : phase functions from an external source

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<i>If AER.Model = 0 : Mie parameters (mono-modal particle model)</i>	
AER.MMD.Mie.FileName	Mie filename written to dirMIE User name or DEFAULT for a default name
AER.MMD.Mie.AlphaMax	Maximum value for size parameter
AER.MMD.MRwa	Real part of the refractive index for the simulation wavelength
AER.MMD.MIwa	Imaginary part of the refractive index (negative value) for the simulation wavelength
<i>If AER.Waref ≠ SOS.Wa</i>	
AER.MMD.MRwaref	Real part of the refractive index for the reference wavelength
AER.MMD.MIwaref	Imaginary part of the refractive index for the reference wavelength
<i>If AER.Model = 0 : parameters of mono-modal size distributions</i>	
AER.MMD.SDtype	Model index 1 : Log-Normal size distribution 2 : Junge law
AER.MMD.SDparam1	Parameter of size distribution If LND : modal radius (µm) If Junge : minimal radius (µm)
AER.MMD.SDparam2	Parameter of size distribution If LND : log10 of variance If Junge : radius exponent
<i>If AER.Model = 1 WMO model</i>	
AER.WMO.Model	WMO model 1 : Continental 2 : Maritime 3 : Urban 4 : User-defined
<i>If AER.WMO.Model = 4 : user concentrations (sum=1)</i>	
AER.WMO.DL	Volumetric concentration of « Dust-Like » components (value between 0 and 1)
AER.WMO.WS	Volumetric concentration of « Water Soluble » components (value between 0 and 1)
AER.WMO.OC	Volumetric concentration of « Oceanic » components (value between 0 and 1)
AER.WMO.SO	Volumetric concentration of « Soot » components (value between 0 and 1)
<i>If AER.Model = 2 : Shettle & Fenn</i>	
AER.SF.Model	Shettle & Fenn model 1 : Tropospheric 2 : Urban 3 : Maritime 4 : Coastal
AER.SF.RH	Percentage of relative humidity (from 0 to 99%)
<i>If AER.Model = 3 :bi-modal LND</i>	
AER.BMD.CVdef	Choice of mixture description type 1 : Use of predefined volumetric concentrations 2 : Use of the ratio of optical thickness of coarse mode over total optical thickness
<i>If AER.BMD.Option= 1 : user-defined volumetric concentrations</i>	
AER.BMD.CoarseVC	volumetric concentration of the coarse mode
AER.BMD.FineVC	volumetric concentration of the fine mode

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<i>If AER.BMD.Option= 2 :</i> Use of ratio coarse mode optical thickness over total AOT	
AER.BMD.RAOT	ratio of coarse mode optical thickness over total one for the reference wavelength.
<i>Coarse mode LND parameters</i>	
AER.BMD.CM.MRwa	Real part of the refractive index for the coarse mode particles at simulation wavelength
AER.BMD.CM.MIwa	Imaginary part of the refractive index for the coarse mode particles at simulation wavelength
AER.BMD.CM.SDradius	Modal radius of LND size distribution for the coarse mode (μm)
AER.BMD.CM.SDvar	Log10 variance of LND size distribution for the coarse mode
<i>If AER.Waref ≠ SOS.Wa</i>	
AER.BMD.CM.MRwaref	Real part of the refractive index for the coarse mode particles at reference wavelength
AER.BMD.CM.MIwaref	Imaginary part of the refractive index for the coarse mode particles at reference wavelength
<i>Fine mode LND parameters</i>	
AER.BMD.FM.MRwa	Real part of the refractive index for the fine mode particles at simulation wavelength
AER.BMD.FM.MIwa	Imaginary part of the refractive index for the fine mode particles at simulation wavelength
AER.BMD.FM.SDradius	Modal radius of LND size distribution for the fine mode (μm)
AER.BMD.FM.SDvar	Log10 variance of LND size distribution for the fine mode
<i>If AER.Waref ≠ SOS.Wa</i>	
AER.BMD.FM.MRwaref	Real part of the refractive index for the fine mode particles at reference wavelength
AER.BMD.FM.MIwaref	Imaginary part of the refractive index for the fine mode particles at reference wavelength
<i>If AER.Model = 4 :</i> phase functions from an external source	
AER.ExtData	Filename of external phase function data (full path)

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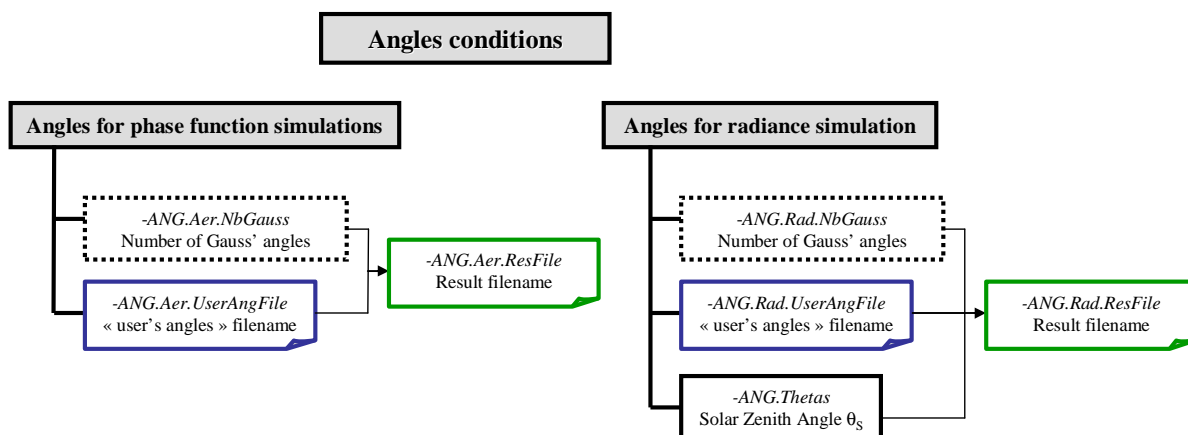
<i>SURFACE CONDITIONS</i>	
SURF.Log	Log file name for SURFACE executable <i>Enter 0 for no log file</i>
SURF.Alb	Surface albedo
SURF.Type	Surface type index 0 : lambertian surface of albedo SURF.Alb 1 : lambertian surface + sunglint (rough sea) 2 : lambertian surface + Fresnel reflection (calm, flat sea) 3 : lambertian surface + Roujean BRDF 4 : lambertian surface + Roujean BRDF + Rondeaux BPDF 5 : lambertian surface + Roujean BRDF + Bréon BPDF 6 : lambertian surface + Roujean BRDF + Nadal BPDF
<i>If SURF.Type = 1 or ≥ 3</i>	
SURF.File	Surface reflection file name <ul style="list-style-type: none"> - File name for user-precomputed Surface reflection matrix (full path). <i>Note : this does not prevent from defining associated parameters that will be useful for analytical calculation of direct reflection.</i> - DEFAULT for a default name (reflection matrix will be generated by the software).
<i>If SURF.Type ≠ 3: for all models except Roujean's</i>	
SURF.Ind	Refractive index surface / air
<i>If SURF.Type = 1 : sunglint</i>	
SURF.Glitter.Wind	Wind speed in m/s
<i>If SURF.Type ≥ 3 : Roujean's BRDF model</i>	
SURF.Roujean.K0	Roujean's model parameter k_0
SURF.Roujean.K1	Roujean's model parameter k_1
SURF.Roujean.K2	Roujean's model parameter k_2
<i>If SURF.Type = 6 : Nadal's BPDF model</i>	
SURF.Nadal.Alpha	Nadal's model parameter α
SURF.Nadal.Beta	Nadal's model parameter β

<i>MOLECULAR SCATTERING PARAMETER</i>	
SOS.MDF	Molecular depolarisation factor

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VIEWING CONDITIONS	
SOS.View	Index of output type 1 : viewing plane 2 : polar diagram (ascii file)
SOS.View.Phi	Relative azimuth angle (degrees) used if SOS.View = 1
SOS.View.Dphi	Azimuth step angles(degrees / integers only) used if SOS.View = 2
CHOICE OF OUTPUT TYPE	
SOS.OutputLevel	Profile level (optional) If not defined : standard output (L _↑ TOA, L _↓ sol) n : upward and downward radiance at profile level n (0 ≤ n ≤ SOS_OS_NT)
SOS.IGmax	Scattering maximum order
SOS.Ipolar	Polarisation truncated index (optional) 0 : simulation of SOS without polarisation If not defined : simulation with polarisation (recommended)
OUTPUT FILE NAMES	
SOS.Log	SOS log file name : <i>Enter 0 for no log file</i>
SOS.ResBin	File name of SOS binary output for Fourier series
SOS.ResFileUp	Ascii file name of the output upward field
SOS.ResFileDown	Ascii file name of the output downward field
SOS.ResFileUp.UserAng	Ascii file name of the output upward field restricted to user-defined angles
SOS.ResFileDown.UserAng	Ascii file name of the output downward field restricted to user-defined angles

III-2.2 Definition of angular conditions



III.2.2.a RADIANCE FIELD SIMULATION PARAMETERS

The Sun's elevation is expressed by its zenith angle θ_s (degrees) : 0 for the Sun at zenith.

The radiance is computed for a discretization of the radiation field with Gauss angles. The user may specify the quadrature order by including the argument *ANG.Rad.NBGauss* directly in the command line (positive μ_G numbers). If not, the value *SOS_DEFAULT_NBMU_LUM* defined by default in *SOS.h* is used.

The user may also define the angles for which radiance values are expected. The file name is given by the argument *-ANG.Rad.UserAngFile*. This file contains a list of angles (degrees) , one record per line.

Example of user-defined angles

```
5.
10.
20.
25.
30.
```

Requirements :

- Angle values must lie between 0 and 90 degrees (in order to define $\mu > 0$ values, opposite values are automatically added by the code).
- Number of records shall not exceed *SOS_NBMAX_USER_ANGLES* (in *SOS.h*).

The user specifies the output file name (*-ANG.Rad.ResFile*). This file contains the angles to be used by the SOS code as well as the maximum orders of the expansions to be applied.

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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 2D 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 G function which acts as a weight factor to the Fresnel matrix during computation of the reflection matrices.
INDEX COS_ANGLE WEIGHT OUTPUT	For each line: angle index, cosine, weight, and whether the angle is a user's defined: (1) if yes, (0) if no. Format: I4,X,2D21.14,X,I4.

Example of an angle file for radiance computation:

NB_TOTAL_ANGLES : 24			
NB_GAUSS_ANGLES : 24			
ANGLES_USERFILE :NO_USER_ANGLES			
SOLAR ZENITH ANGLE : 32.479			
INTERNAL_IMUS : 9			
INTERNAL_OS_NB : 80			
INTERNAL_OS_NS : 48			
INTERNAL_OS_NM : 128			
INDEX	COS_ANGLE	WEIGHT	OUTPUT
1	0.99877100725243E+00	0.31533460522976E-02	0
2	0.99353017226635E+00	0.73275539012758E-02	0
3	0.98412458372283E+00	0.11477234579235E-01	0
4	0.97059159254625E+00	0.15579315722944E-01	0
5	0.95298770316043E+00	0.19616160457356E-01	0
6	0.93138669070655E+00	0.23570760839325E-01	0
7	0.90587913671557E+00	0.27426509708357E-01	0
8	0.87657202027425E+00	0.31167227832799E-01	0
9	0.84358826162439E+00	0.34777222564771E-01	0
10	0.80706620402944E+00	0.38241351065831E-01	0
11	0.76715903251574E+00	0.41545082943465E-01	0
12	0.72403413092381E+00	0.44674560856694E-01	0
13	0.67787237963266E+00	0.47616658492491E-01	0
14	0.62886739677651E+00	0.50359035553855E-01	0
15	0.57722472608397E+00	0.52890189485194E-01	0
16	0.52316097472223E+00	0.55199503699984E-01	0
17	0.46690290475096E+00	0.57277292100403E-01	0
18	0.40868648199072E+00	0.59114839698396E-01	0
19	0.34875588629216E+00	0.60704439165894E-01	0
20	0.28736248735546E+00	0.62039423159893E-01	0
21	0.22476379039469E+00	0.63114192286254E-01	0
22	0.16122235606889E+00	0.63924238584648E-01	0
23	0.97004699209463E-01	0.64466164435950E-01	0
24	0.32380170962869E-01	0.64737696812684E-01	0

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III.2.2.b PHASE FUNCTION PARAMETERS

The same settings as above are offered for the processing of aerosol properties.

The SOS_ANGLES program generates a file for angles and expansion orders used for the determination of aerosol phase functions.

The file contains the following information :

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,X,2D21.14,X,I4.	
•		
•		
•		

Example of files with angles for determination of aerosol radiative properties:

```

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
12 0.43387537083176E+00 0.35160529044748E-01
13 0.46869661517054E+00 0.34473120451754E-01
14 0.50280411188878E+00 0.33733214984612E-01
15 0.53614592089713E+00 0.32941939397646E-01
16 0.56867126812271E+00 0.32100498673488E-01
17 0.60033062282975E+00 0.31210174188115E-01
18 0.63107577304687E+00 0.30272321759558E-01
19 0.66085989898612E+00 0.29288369583267E-01
20 0.68963764434203E+00 0.28259816057277E-01
21 0.71736518536210E+00 0.27188227500486E-01
22 0.74400029758360E+00 0.26075235767565E-01
23 0.76950242013504E+00 0.24922535764116E-01
24 0.79383271750461E+00 0.23731882865930E-01
25 0.81695413868146E+00 0.22505090246332E-01
26 0.83883147358026E+00 0.21244026115782E-01
27 0.85943140666311E+00 0.19950610878142E-01
28 0.87872256767821E+00 0.18626814208300E-01
29 0.89667557943877E+00 0.17274652056270E-01
30 0.91326310257176E+00 0.15896183583725E-01
31 0.92845987717245E+00 0.14493508040509E-01
32 0.94224276130987E+00 0.13068761592400E-01
33 0.95459076634363E+00 0.11624114120797E-01
34 0.96548508904380E+00 0.10161766041103E-01
35 0.97490914058573E+00 0.86839452692619E-02
36 0.98284857273863E+00 0.71929047681184E-02
37 0.98929130249976E+00 0.56909224514043E-02
38 0.99422754096569E+00 0.41803131246912E-02
39 0.99764986439824E+00 0.26635335895143E-02
40 0.99955382265163E+00 0.11449500031887E-02

```

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III-2.3 Surface conditions

The SOS code may simulate various model of homogeneous surfaces : sea surface with or without waves, lambertian land surfaces, or surfaces with BRDF/ BPDF.

III.2.3.a SEA SURFACES

The sea surface is characterized by a lambertian term of diffuse reflectance and by a directional term of specular reflection of the direct and scattered solar radiation illuminating the sea. The properties of surface reflection are characterized by Fresnel's laws. They depend on the refractive index of water (real value in the visible domain) and on the slope of the waves. The software allows to simulate the case of a calm flat sea (no wind) and the case of a rough sea for which wave slope statistics is function of wind speed (sunglint case) [cf. DR5, DR9].

III.2.3.b LAND SURFACES

The SOS code simulates light reflection on a flat surface. Reflectance may be Lambertian or may follow a law of directional reflection with intensity (BRDF) or polarisation (BPDF).

It is possible to simulate the BRDF of a vegetation cover or of a bare land according to Roujean's model [DR14]. Only 3 parameters (k_0 , k_1 , k_2) are necessary to characterize this model. They are estimated by the user with respect to the surface conditions he wishes to simulate. These parameters are dependant on the nature of the surface. Their values must have a dimension allowing to simulate reflectance.

BPDF available models are :

- Rondeaux's model allows to simulate vegetation polarisation [DR13],
- Bréon's model is well-defined for polarisation of bare surfaces [DR2],
- Nadal's semi-empirical model [DR12] is function of two parameters α and β .

We have chosen Roujean's model for the BRDF associated to these models (BRDF is added to the intensity term of the polarisation reflection matrix).

These models require the refractive index of surface / air for the determination of Fresnel's reflection.

III.2.3.c FILES FOR SURFACE REFLECTION MATRICES

The computation of a surface reflection matrix is time-consuming and often redundant from one simulation to another. Therefore, it was decided to write the estimated surface reflection matrices to disk and save them instead of recomputing them every time. The output matrices are saved in a directory defined by the user in the script runOS.ksh.

The SOS_SURFACE application generates reflection matrices for the models. In the case of a simulation of type BRDF / BPDF, the user may define the output file named SURFACE. The user may also let the application pick a name by entering DEFAULT instead. The file name will then be defined with respect to the simulation parameters. For example, in the case of sunglint simulations, the file name will depend on the water index, wind speed and viewing angles according to the pattern « **GLITTER**-index-wind-MUnnn-ficUser ». For a water index of 1.5, a wind speed of 12.5 m.s^{-1} and working with 24 Gauss angles completed by a user-defined angle files named « MyAngles » (independently of its location), the output filename will be « GLITTER-1.500-12.5-MU24-MyAngles ». The application verifies if the file already exists and if it does, it does not recompute it.

Caution :

- Even if physically correlated, the values of the surface physical parameters and the value of the simulation wavelength are defined independently in the file runOS.ksh. The user must make sure they are consistent.
- A change in the user-defined angles without change of filename does not lead to reprocessing of the file SURFACE. The user must change the names of the modified angle files or suppress the existing SURFACE files in order to avoid simulation errors.
- In the case user-defined angles are being used, the output SURFACE files indicates the basename of the input angle file without its path. It is recommended to use one unique folder for angle files and/or to apply a rigorous filenames convention.

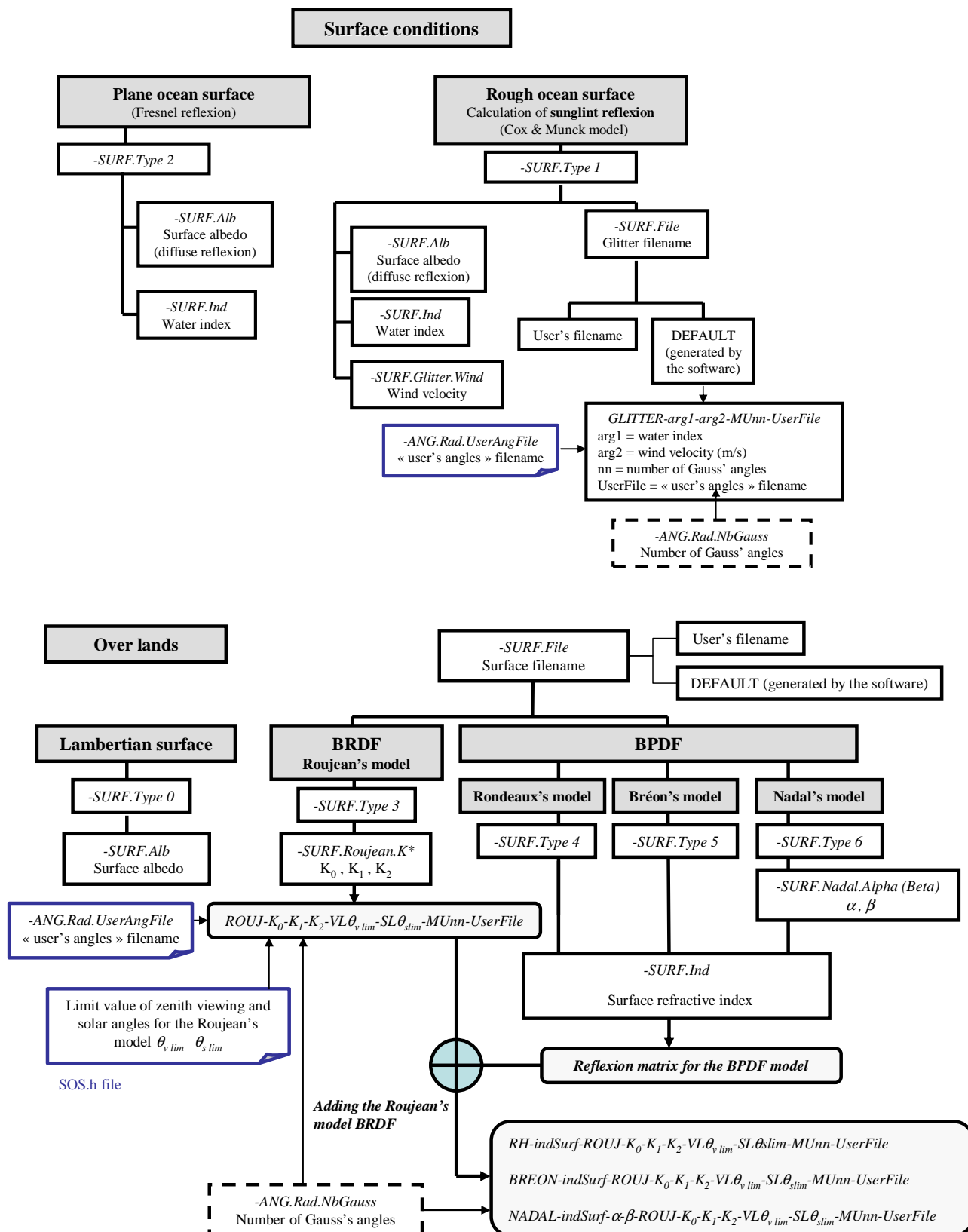
Table 2 : Format of parameters relative to the file naming convention used for SURFACE files

Parameter	Bounds	Last significant digit	Associated format
Wind speed	$< 100 \text{ m.s}^{-1}$	Numerical error is $\sim 10^{-1}$	F4.1
Surface index		Numerical error is $\sim 10^{-3}$	F5.3
K_0, K_1, K_2 from Roujean's model			F7.3
α from Nadal's model		Numerical error is $\sim 10^{-4}$	F6.4
β from Nadal's model		Numerical error is $\sim 10^{-1}$	F4.1

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Table 3 : Format of parameters relative to the file naming convention used for SURFACE files

Type of surface	Associated name
Roujean's model	ROUJ-k0-k1-k2-VL-SL-MU_{nnn}-ficUser NB : VL, SL are constant values defined in SOS.h (limits of viewing and solar angles). nnn : number of Gauss angles ficUser : filename of user-defined angles (optional) Ex : ROUJ-000.243-000.073-000.642-VL60-SL60-MU24
Rondeaux' model	RH-indSurf-ROUJ-k0-k1-k2-VL-SL-MU_{nnn}-ficUser Ex : RH-1.500-ROUJ-000.243-000.073-000.642-VL60-SL60-MU24
Bréon' model	BREON-indSurf-ROUJ-k0-k1-k2-VL-SL-MU_{nnn}-ficUser Ex : BREON-1.500-ROUJ-000.243-000.073-000.642-VL60-SL60-MU24
Nadal's model	NADAL-indSurf-α-β-ROUJ-k0-k1-k2-VL-SL-MU_{nnn}-ficUser Ex : NADAL-1.500-0.0229-38.0-ROUJ-000.243-000.073-000.642-VL60-SL60-MU24

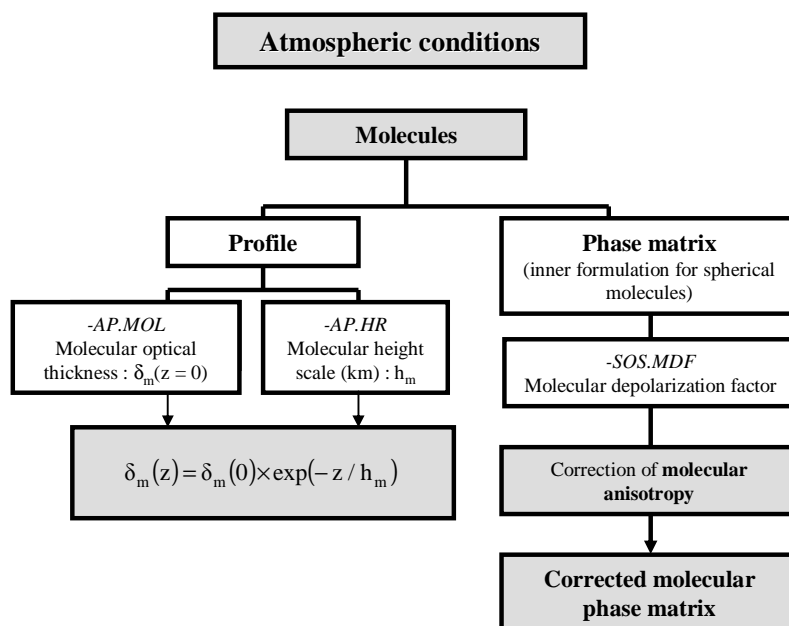


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III-2.4 Atmospheric conditions

The SOS code computes light propagation in a scattering atmosphere by clear sky. The atmospheric components considered are molecules and aerosols. Gaseous absorption is not considered.

III.2.4.a MOLECULAR DIFFUSION



Molecular scattering depends on the profile of atmospheric pressure and of the considered wavelength. Instead of using the optical thickness computed by the application, for a given pressure and wavelength, the user may enter the molecular optical thickness (integrated over the atmospheric column). As such, the user may simulate the inherent radiation of an aerosol layer by suppressing the molecular component with a null optical thickness.

The pressure profile is estimated by a decreasing exponential $\exp(-z / h_m)$, characterized by a height scale h_m (typically 6 to 8 km). Molecular scattering properties are well-known and implemented by the SOS code. Molecular anisotropy is considered in terms of a depolarisation factor [DR9]. By default the proposed value for this factor is 0,0279.

The molecular optical thickness may be estimated according to the classical equation of Hansen & Travis [DR8] at the surface level and for a standard atmospheric pressure of 1013 mb :

$$\tau_m = \left(\frac{84,35}{\lambda^4} + \frac{-1,225}{\lambda^5} + \frac{1,4}{\lambda^6} \right) \times 10^{-4} \text{ for } \lambda \text{ in } \mu\text{m} \quad (1)$$

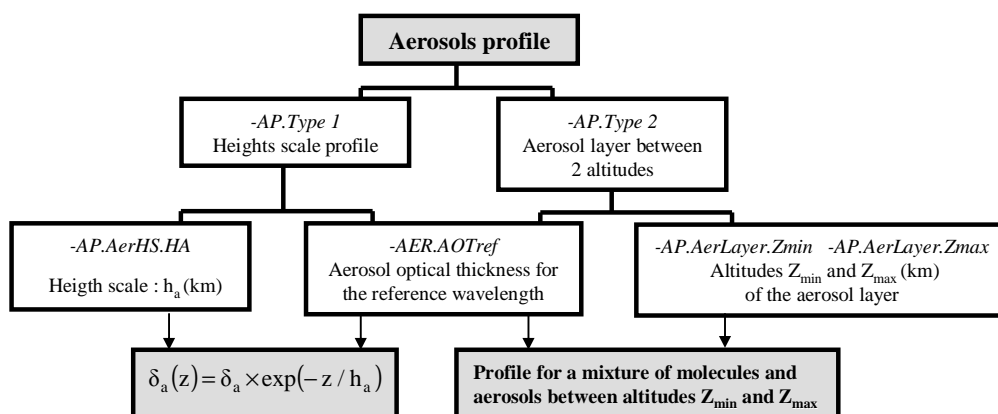
The more recent formalism by Bodhaine et al. [DR1], which takes into account the increase of carbon dioxide, could lead to a better estimation.

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III.2.4.b AEROSOL DIFFUSION AND ABSORPTION

• *Aerosol vertical profile :*

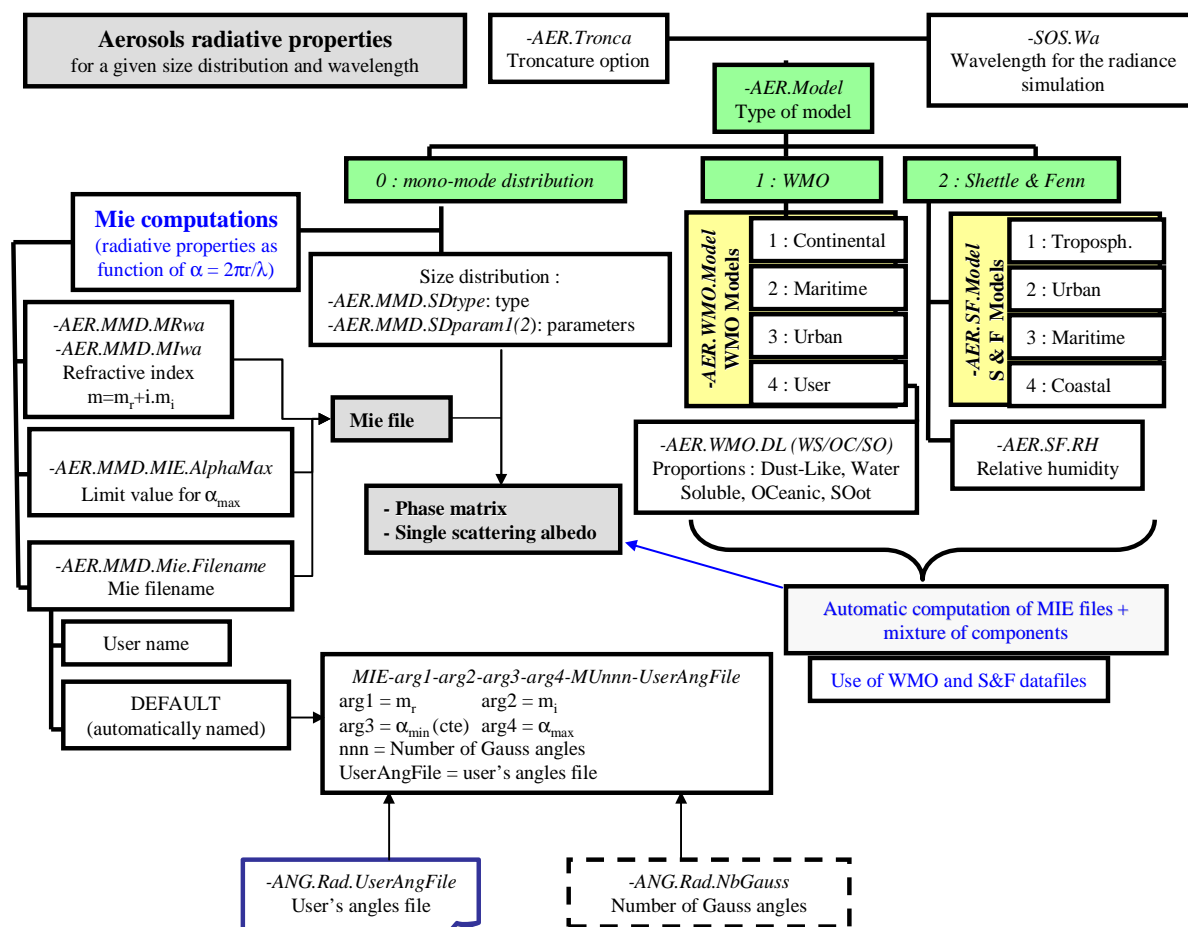
The aerosol vertical profile may be characterized by an exponential decrease of the optical thickness $\exp(-z / h_a)$, with a typical height scale h_a of about 2km. The user may simulate an aerosol layer (homogeneous mixture of molecules and aerosols) between 2 pure molecular layers. The total aerosol optical thickness, τ_a , depends on the type and abundance of particles for a given wavelength λ . Its value is defined by the user. It is possible to simulate pure scattering by setting $\tau_a = 0$.

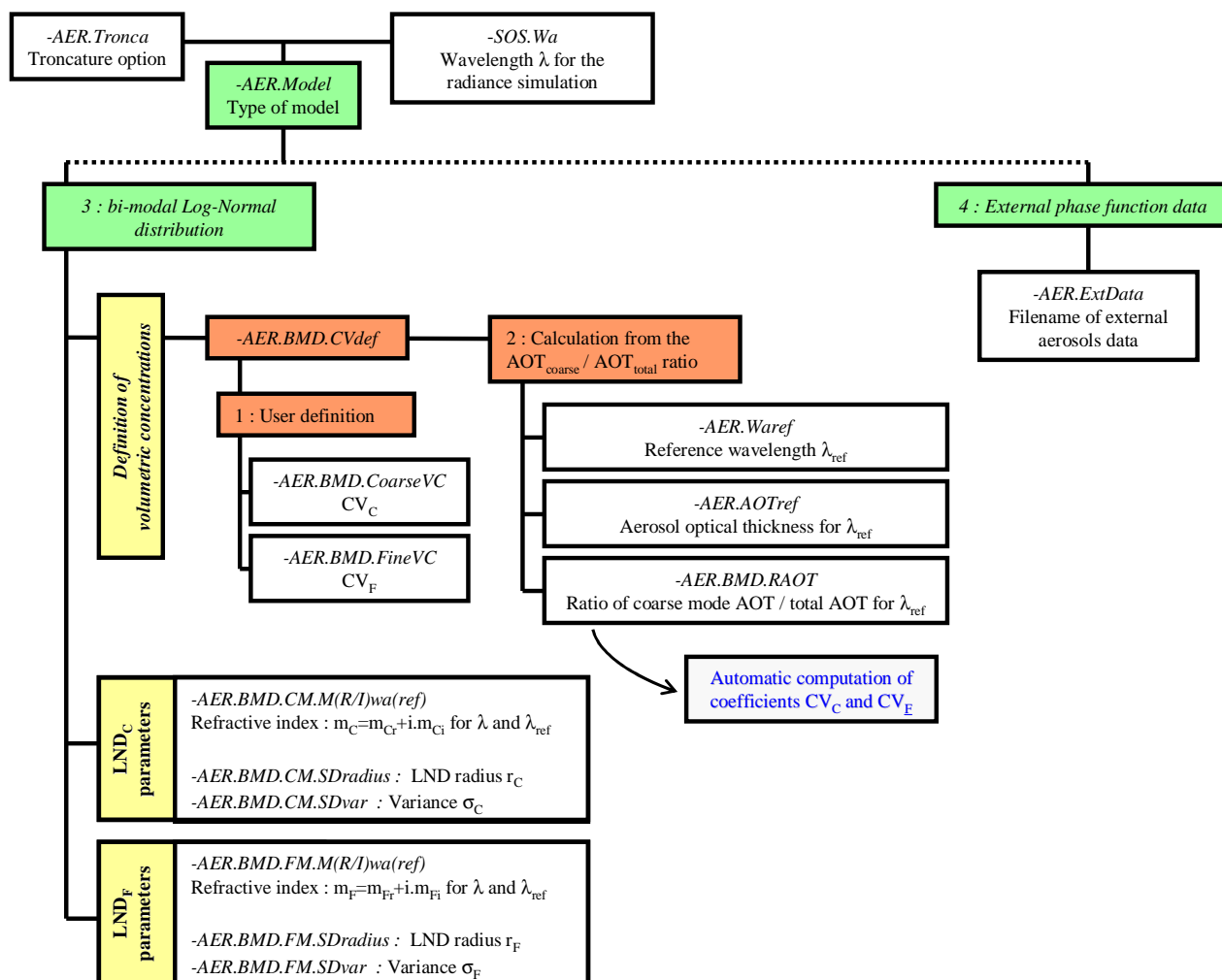


• *Aerosol model :*

Aerosol radiative properties can be defined as :

- The user may select a model type : it is possible to simulate mono-modal size distributions (log-normal law or Junge law) as well as more complex models such as bi-modal distributions or predefined models from WMO [DR19] or Shettle & Fenn [DR15] (continental, urban, maritime and coastal models considering the air relative humidity).
- The user may use a file of external phase functions, which allows to simulate scattering of non-spherical particles (with random orientation, so as to consider the symmetry of the radiation field about the main solar plane). The content and format of this file are given in section §III.2.4.c, p. 39.
- The user may also reuse the output file of a previous run from SOS_AEROSOLS (giving the scattering and extinction coefficients, and the decomposition coefficients of the phase matrix). The content and format of this file are given in section §III.2.4.d, p. 41.





The radiative properties of an aerosol specie are computed for a size distribution $N(r)$ and wavelength λ . Aerosols are considered spherical. Their chemical nature is defined by their refractive index $m = m_r + i.m_i$ ($m_i \leq 0$ for absorption), assuming an homogeneous composition.

Mie's theory allows to estimate radiative properties of a spherical particle of radius r and index m , for an incident radiation of wavelength λ . Mie's equations are solved in terms of the size parameter $\alpha = 2.\pi.r / \lambda$, in the range α_{\min} to α_{\max} . The solution is then applied to the size distribution $N(r)$ in order to estimate the radiative properties at the macroscopic scale for the particle distribution and for the wavelength of interest.

Mie's processing is time-consuming. The output is saved to disk in a user-specified directory. If the file already exists (same name), it is not recomputed. In the case of a mono-modal distribution, the user may either define the output file name of the SOS_AEROSOLS application, or let the software define it automatically by typing DEFAULT. If the user simulates a bi-modal or multi-modal model of WMO [DR19] or Shettle & Fenn [DR15], the file naming convention for Mie's output files is applied automatically by the software (i.e. the user can not define the name of the output file). The pattern for Mie's output filenames is based on the refractive index, the parameters for size limits, the number of used Gauss' angles (nnn) and may include the name of the file for user-defined angles ($ficUser$ base name). It is such as **MIE**- m_r - $|m_i|$ - α_{\min} - α_{\max} -**MU** nnn - $ficUser$. The precision associated to each parameter is given in the table below.

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Tableau 4 : Format of parameters relative to the filnaming convention for MIE's files.

Parameter	Range	Precision	Format	Pattern
m_r		Error is 10^{-3}	F5.3	x.xxx (ex : $m_r=1.53 \Rightarrow 1.530$)
m_i	< 0	Error is 10^{-5}	F8.5	x.xxxxx (ex : $m_i=-0.008 \Rightarrow 0.002800$)
α_{\min}	$10^{-4} < \alpha_{\min} < 10$	Error is 10^{-4}	F6.4	x.xxxx (ex : $\alpha_{\min} = 0.0001 \Rightarrow 0.0001$)
α_{\max}	$10^{-2} < \alpha_{\max} < 10^5$	Error is 10^{-2}	F9.2	xxxxx.xx (ex : $\alpha_{\max} = 500 \Rightarrow 00500.00$)

For example, for an index $m = 1,53 - i \times 0,008$ and solving from $\alpha_{\min} = 0,0001$ to $\alpha_{\max} = 500$ using 40 Gauss angles, the output file is named : « MIE-1.530-0.00800-0.0001-00500.00-MU40 ».

Caution :

- The value of the molecule optical thickness is defined in the file runOS.ksh, the user must make sure that it is consistent with the wavelength selected for the radiance simulation.
- A change in the user-defined angles without change of filename does not lead to reprocessing of the file MIE. The user must change the names of the modified angle files or suppress the existing MIE files in order to avoid simulation errors.
- In the case user-defined angles are being used, the output MIE files indicates the base name of the input angle file without its path. It is recommended to use one unique folder for angle files and/or to apply a rigorous file naming convention.

•Definition of aerosol properties for a reference wavelength :

The user defines the following aerosol properties :

- for a reference wavelength :
 - the optical thickness of aerosol,
 - the refractive index (real and imaginary part) for each mode of particles.
- For the wavelength of the radiation field simulation :
 - the refractive index (real and imaginary part) for each mode of particles.

The application computes the extinction coefficients of the model for both the reference wavelength and the wavelength of the radiation field simulation. The aerosol optical thickness for the simulation wavelength is then deduced by:

$$\tau_{\lambda_{\text{simu}}} = \tau_{\lambda_{\text{ref}}} \times \frac{\sigma_{\lambda_{\text{simu}}}^{\text{ext}}}{\sigma_{\lambda_{\text{ref}}}^{\text{ext}}}$$

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• ***Truncation of the aerosol phase function:***

When the scattering particles are large, scattering occurs mainly forward within an opened cone of few degrees. This strong anisotropy of the scattering effect makes the mathematical formulation of the phase function more difficult. Physically, the radiation scattered forward can not be uncoupled from the transmitted radiation. We may consider that the energy scattered at small angles is equivalent to a transmitted energy. The phase function part related to small scattering angles may then be truncated which allows to reduce the number of terms in its expression by Legendre Polynomials and therefore to reduce the computation time.

Truncating the phase function modifies the energy distribution. The other radiative parameters, which describe the atmospheric layer, must then be adjusted so that the global radiative properties remain unchanged.

It is highly recommended that the user systematically asks for truncation. The physical values entered in the file runOS.ksh must not be truncated. The software program is in charge of truncating the phase function and adjusting the radiative parameters as necessary. The output results are equivalent to what would have been obtained without truncation but the processing is much faster (i.e, the same results could be obtained without truncation but for an expansion of the phase function with much more coefficients, which involves using a quite higher Gauss' quadrature).

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III.2.4.c FILE FORMAT OF THE EXTERNAL PHASE FUNCTIONS

The format of this file is compatible with the tool named DLS of Oleg Dubovik [DR7] which provides the primary scattering properties of homogeneous spheroid particles with random orientation. However, a parameter defining the number of angles describing the functions was added.

It consists of an Ascii file with the following records :

1st line : **ext=Value abs=Value sca=Value**

format : FORMAT(4hext=,E15.5,4habs=,E15.5,4hsca=,E15.5)

Values : ext : extinction coefficient

 abs : absorption coefficient

 sca : scattering coefficient

Note : the only parameters used by the SOS code are the extinction (ext=) and scattering (sca=) coefficients.

2nd line : **nbAng=Value**

format : FORMAT(6hnbAng=,I4)

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

It can not exceed the value **SOSMAXNB_ANG_EXT** (in SOS.h).

3rd line : Comments

Lines 4 to (4+nbAng-1) : **ANGLE F11 -F12/F11 F22/F11 F33/F11**

format : FORMAT(F7.2,6E14.5)

Value: ANGLE : 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 code.

The next lines are not read.

Example of file for external phase functions

```

ext= 0.72684E+00  abs= 0.49962E-01  sca= 0.67688E+00
nbAng= 181
  ANGLE      F11      -F12/F11      F22/F11      F33/F1
    0.00    0.38325E+03    0.00000E+00    0.99984E+00    0.99984E+0
    1.00    0.27348E+03    0.83746E-04    0.99978E+00    0.99978E+00
    2.00    0.15766E+03    0.23956E-03    0.99963E+00    0.99962E+0
    3.00    0.91944E+02    0.39548E-03    0.99938E+00    0.99932E+0
    4.00    0.56217E+02    0.62078E-03    0.99903E+00    0.99882E+0
    5.00    0.36374E+02    0.10123E-02    0.99855E+00    0.99809E+0
    6.00    0.24931E+02    0.16408E-02    0.99793E+00    0.99712E+0
    7.00    0.18065E+02    0.25726E-02    0.99719E+00    0.99592E+0
    8.00    0.13797E+02    0.38248E-02    0.99633E+00    0.99456E+0
    9.00    0.11049E+02    0.53602E-02    0.99538E+00    0.99312E+0
  .
  .
  .
 167.00    0.18637E+00   -0.10822E-01    0.76091E+00   -0.69151E+00
 168.00    0.18857E+00   -0.10740E-01    0.76193E+00   -0.69161E+00
 169.00    0.19077E+00   -0.10116E-01    0.76338E+00   -0.69214E+00
 170.00    0.19288E+00   -0.86482E-02    0.76494E+00   -0.69391E+00
 171.00    0.19502E+00   -0.61878E-02    0.76614E+00   -0.69759E+00
 172.00    0.19753E+00   -0.27749E-02    0.76622E+00   -0.70338E+00
 173.00    0.20101E+00    0.13766E-02    0.76422E+00   -0.71097E+00
 174.00    0.20629E+00    0.54762E-02    0.75934E+00   -0.71884E+00
 175.00    0.21404E+00    0.83942E-02    0.75137E+00   -0.72485E+00
 176.00    0.22441E+00    0.90428E-02    0.74083E+00   -0.72721E+00
 177.00    0.23650E+00    0.65456E-02    0.72965E+00   -0.72470E+00
 178.00    0.24726E+00    0.22419E-02    0.72103E+00   -0.71917E+00
 179.00    0.25198E+00    0.18433E-04    0.71772E+00   -0.71611E+00
 180.00    0.25674E+00    0.00000E+00    0.71376E+00   -0.71240E+00

```


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III.2.4.d CONTENT AND FORMAT OF A FILE OF TYPE AEROSOLS FOR THE SOS CODE

An “Aerosol” file for the SOS code is a formatted Ascii file. It is organized as follows :

$\tilde{\sigma}_e$	$\tilde{\sigma}_d$	g	
A			
ω_0			
α_0	β_0	γ_0	ξ_0
α_1	β_1	γ_1	ξ_1
\vdots	\vdots	\vdots	\vdots
α_{OS_NB}	β_{OS_NB}	γ_{OS_NB}	ξ_{OS_NB}

1st line : general information (values are not adjusted with respect to truncation)

- Extinction cross-section (μm^2),
- Scattering cross-section (μm^2),
- Asymmetry factor ($g = \beta_1 / 3$).

Format : 2(2X, E13.5), E13.5

Note : the data of this first line are for information purpose only. They are read but not utilized by the SOS code except for the extinction cross-section which is used by the main script main_SOS.ksh for computing the aerosol optical thickness for the wavelength of radiation field simulation derived from the AOT of the reference wavelength.

2nd ligne : truncation coefficient A (null if the phase function is not truncated).

Format : 2X, F9.5

3^{ème} ligne : Single scattering albedo (may be truncated if $A \neq 0$).

Format : 2X, F9.5

Next lines : Coefficients of the phase matrix $\alpha_k, \beta_k, \gamma_k, \xi_k$ (may be truncated if $A \neq 0$) for $k = 0$ to OS_NB (maximum order of development defined in the ANGLES file and correlated to the number of Gauss' angles).

Format : 4(2X, E16.8)

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III-2.5 Type of output

- The simulation output is a **scattered field of radiance normalized** by the solar irradiance. Let L^* be the radiance and E_s the solar irradiance, the normalized radiance is then : $L = \pi \times L^* / E_s$ (the reflectance is $\rho = L / \cos \theta_s$).

- **Output level in the atmospheric profile for the normalized radiance field:**

The normalized radiance field is computed for a range of atmospheric profile levels. The outputs are the upward and downward radiance for the selected level. The user may specify :

- the output level of the radiance field :
 - Enter `SOS.OutputLevel = -1` for generating the upward radiance at Top of atmosphere (TOA) and downward incidence at ground level,
 - Enter `SOS.OutputLevel = n` with $0 \leq n \leq \text{SOS_OS_NT}$ for the output radiance at level n : 0 for TOA, `SOS_OS_NT` for the ground (constant parameter defined in `SOS.h`),
- The name of the output files :
 - File name of the upward radiance.
 - File name of the downward radiance.

- **Neglecting polarisation :**

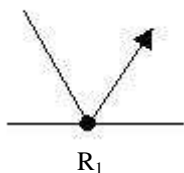
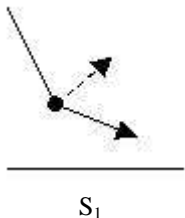
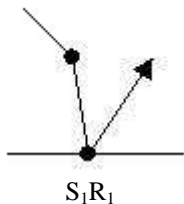
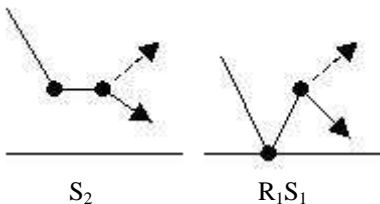
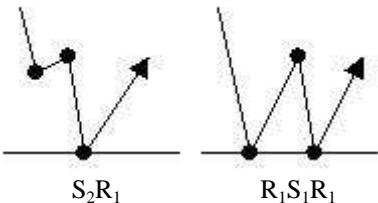
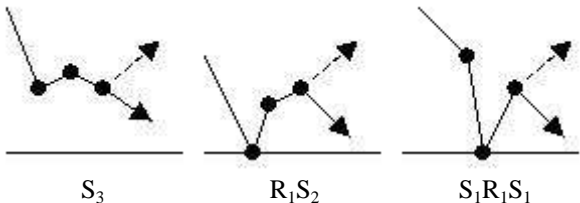
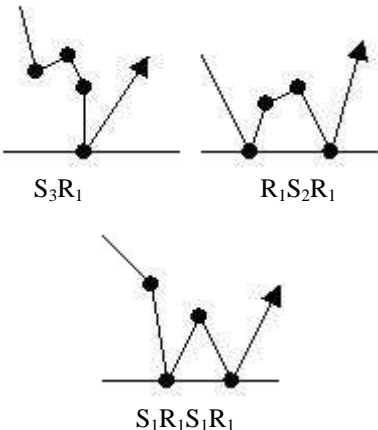
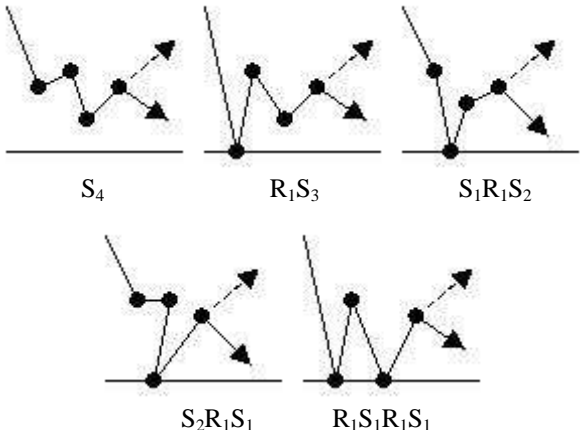
One main specificity of the SOS code is to simulate the light polarisation. It is nonetheless possible to perform a simulation without taking into account polarisation effects. Polarisation is then neglected in the propagation of radiation by the SOS code, but this simplification does not affect the MIE files or BPDF files of surface products.

- **Maximum order of interactions**

The SO code, as its name suggests, follows the successive orders of interaction (scattering and reflections). The user may specify the maximum order « `SOS.IGmax` » above which no computation will be performed. The nominal number of orders of interactions is determined by the code according to a convergence criterion which checks whether the next interactions are significant enough. Typically convergence is reached within a few scattering interactions. For usual AOT, the user may set `SOS.IGmax > 20` to let the code stops automatically according to the convergence criterion. On the other hand, if the user wishes to validate each successive interaction, he may set `SOS.IGmax` to 1, 2, 3 ...

Table 5 illustrates the first orders of interaction.

Table 5 : terms of order ig computed by the SOS code. The left column illustrates the upward radiance at the ground, the right column the downward radiance. At TOA, one finds the term of surface reflection (left column) attenuated and the atmospheric scattering term (right column) for a scattering effect upwards.

Ig	Upward light at ground level	Downward light at ground level or upward at TOA
1	 R_1	 S_1
2	 S_1R_1	 S_2 R_1S_1
3	 S_2R_1 $R_1S_1R_1$	 S_3 R_1S_2 $S_1R_1S_1$
4	 S_3R_1 $R_1S_2R_1$ $S_1R_1S_1R_1$	 S_4 R_1S_3 $S_1R_1S_2$ $S_2R_1S_1$ $R_1S_1R_1S_1$

• **Transmissions :**

On user request, the SOS code provides transmissions corresponding to the simulated atmosphere (for the true optical thickness and not the one resulting from a truncation of the aerosol phase function) :

- Direct transmission from TOA to ground for the solar incidence.
- Diffuse transmission from TOA to ground for the solar incidence.
- Diffuse transmission from ground to TOA for all viewing angles.

• **Viewing conditions :**

SOS computations are performed for all the Gauss angles and additional angles of the optional list defined by the user. The radiance field is provided for all the angles or only for the user-defined angles (option).

Expansion in Fourier series, performed with respect to the relative azimuth between the solar direction and the viewing direction, allows retrieving the simulated radiance for any direction in azimuth. The user may request the simulated radiance for one given azimuth plane or for a set of azimuthal directions.

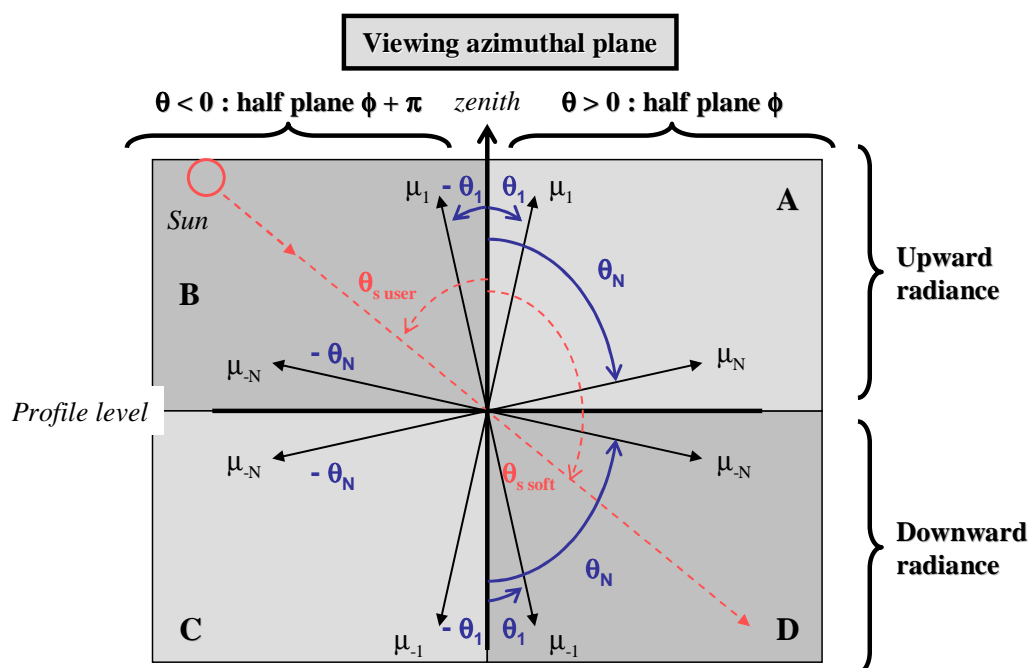
Case 1 : Output is a viewing plane

If the user wants the output for a given azimuthal plane, it sets the corresponding flag `SOS.View = 1` and defines the value of the relative azimuth angle ϕ .

The output files then give the normalized radiance corresponding to the Gauss angles defined in the input file.

Convention :

- Sign of angles :
 - The viewing angle is positive in the half-plane of relative ϕ .
 - It is negative in the half-plane $\phi + \pi$.
- 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 $\pm 90^\circ$ for the horizon.

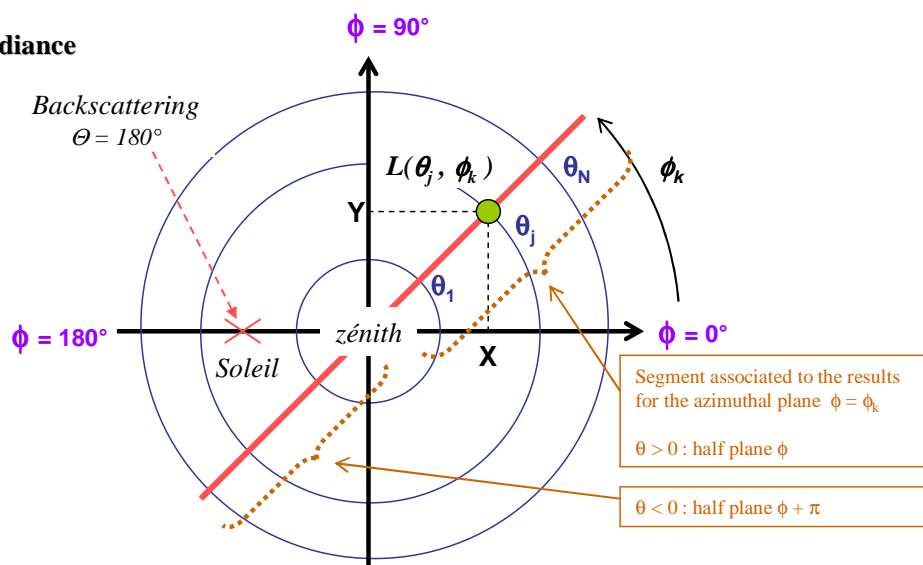
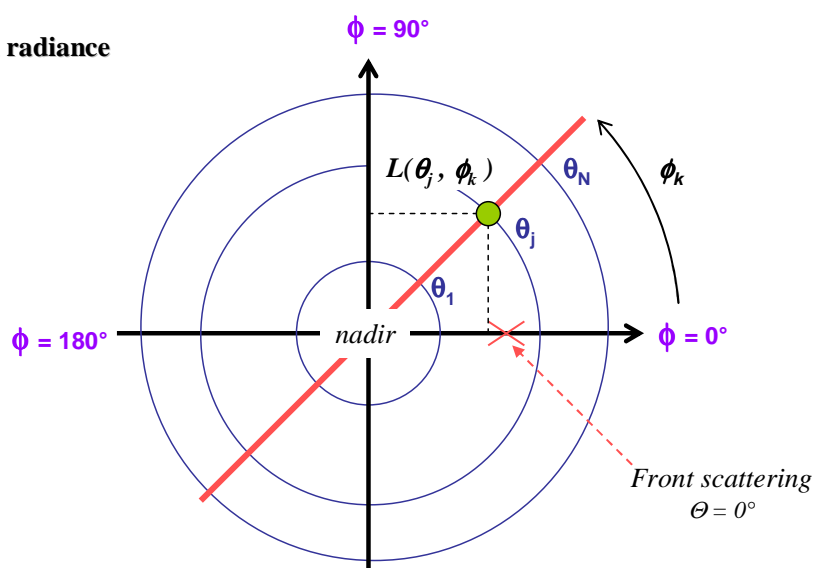


Case 2 : Output for a set of azimuthal directions

It is possible to obtain a full output of the upward and downward radiance for the selected profile level (SOS.View = 2). The user must specify the sampling step in azimuth : $\Delta\phi$ (integer value).

The output files contain 5 columns:

- 1st column : $X = \phi$
- 2nd column : $Y = \theta_v > 0$ (unsigned zenith angle for the upward field, angle defined with respect to nadir for the downward field)
- 3rd to 5th column : $Z_I = I(\theta_v, \phi)$ $Z_Q = Q(\theta_v, \phi)$ $Z_U = U(\theta_v, \phi)$

Illustration of radiance field of view**Upward radiance****Downward radiance**

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III-2.6 Output files

The software application generates several types of files:

- **Files forming a “data base”** (if automated file naming) – the full path is specified by the user :
 - Files containing the Fourier series of the reflection matrices,
 - Files containing MIE’s computations.
- **Temporary files** which are automatically removed at the end of the processing :
 - « RES_FRESNEL » : expansion of the Fresnel matrix in Fourier series,
 - « RES_GSF » : Fourier series of the G function relative to the surface model and used as weighting function of the Fresnel matrix.
 - « RES_MAT_REFLEX » : expansion in Fourier series of the surface reflection matrix,
 - « *_BPDF » : BPDF results before the contribution of Roujean’s BRDF.
- **Input files to SOS, simulation-specific** (replaced at each simulation) :
 - Files containing angles and orders of expansion being processed,
 - Atmospheric profile of the optical thickness,
 - Description of the radiative properties of the aerosol model.
- **SOS output files** : Final simulation results.
 - Binary file for the upward and downward polarized field decomposed as Fourier series,
 - Ascii file of the upward field for all angles or for user-defined angles only.
 - Ascii file of the downward field for all angles or for user-defined angles only.
 - Ascii file for diffuse and direct transmissions.
- **Log files** : they record information relative to each step. These files may be very large, so it is recommended to generate them only if necessary.

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III-2.7 Example of launch file : Simulation over the ocean

Let suppose that we would like to simulate the sunglint reflection at 440 nm for a wind speed of 2 m.s^{-1} , an ocean albedo of 0.02 and a water refractive index of 1.34. The atmosphere is supposed slightly turbid with an aerosol optical thickness of 0.05 at 550-nm, index 1.4 (non absorbing) at 440 nm and 1.45 at 550 nm, of log-normal size-distribution (modal radius r_m equal to $0.3 \mu\text{m}$ and variance σ such that $\log_{10}(\sigma) = 0.4$). We will request the phase function to be truncated. The aerosol layer will extend from the ground to TOA with an exponential decrease of the optical thickness. The molecular optical thickness is 0.23 at 440 nm. The zenith solar angle is 30° . We want to generate a global radiation field emerging at TOA and illuminating the ground, by step of 5 degrees in relative azimuth. We would also like to output the transmission values.

```

$RACINE/exe/main_SOS.ksh -SOS.Wa 0.440 \
-ANG.Rad.NbGauss 24 -ANG.Rad.ResFile ${dirRESULTS}/SOS_UsedAngles.txt \
-ANG.Aer.NbGauss 40 -ANG.Aer.ResFile ${dirRESULTS}/AER_UsedAngles.txt \
-ANG.Log ${dirLOG}/Angles.Log \
-ANG.Thetas 30. -SOS.View 2 -SOS.View.Dphi 5 \
-SOS.IGmax 30 \
-SOS.ResFileUp ${dirRESULTS}/SOS_Up.txt -SOS.ResFileDown ${dirRESULTS}/SOS_Down.txt \
-SOS.ResBin ${dirRESULTS}/SOS_Result.bin \
-SOS.Log ${dirLOG}/SOS.Log \
-SOS.Config ${dirRESULTS}/SOS_config.txt \
-SOS.Trans ${dirRESULTS}/SOS_transm.txt \
-AP.ResFile ${dirRESULTS}/Profile.txt -AP.Log ${dirLOG}/Profile.Log \
-AP.MOT 0.230 -SOS.MDF 0.0279 \
-AP.Type 1 -AP.HR 8.0 -AP.AerHS.HA 2.0 \
-AER.Waref 0.550 -AER.AOTref 0.05 \
-AER.ResFile ${dirRESULTS}/Aerosols.txt -AER.Log ${dirLOG}/Aerosols.Log -AER.MieLog 0 \
-AER.Tronca 1 -AER.Model 0 \
-AER.MMD.Mie.AlphaMax 300 -AER.MMD.MRwa 1.4 -AER.MMD.MIwa 0. \
-AER.MMD.MRwaref 1.45 -AER.MMD.MIwaref 0. \
-AER.MMD.SDtype 1 -AER.MMD.SDparam1 0.3 -AER.MMD.SDparam2 0.4 \
-SURF.Log ${dirLOG}/Surface.Log -SURF.File DEFAULT \
-SURF.Type 1 -SURF.Alb 0.02 -SURF.Ind 1.34 \
-SURF.Glitter.Wind 2.0

```

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III-3 Constant parameters of the simulation

III-3.1 List of constant parameters included in SOS.h

Along with the physical simulation parameters that we have just seen, we also need to define some more processing parameters. These parameters deal with the size of 2D-arrays used in the code, as well as with threshold values required for the convergence criteria. These parameters are defined at compile time via the include file **SOS.h** (under \$RACINE/inc). Their modification requires a good understanding of how the software works.

Caution : A change to a constant value will only be effective after the software has been recompiled.

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Table 6 : software constant values

Constant values		SOS.h
Name	Description	Default value
1) Constant values shared by all programs		
SOS_LENDIR	Maximum length of strings for directory names.	150
SOS_LENFC1	Maximum length of strings for file names (basename only).	150
SOS_LENFC2	Maximum length of strings for files with full path	300
SOS_LENKEYWORD	Maximum length of Keywords for the arguments	30
SOS_PI	π	3.14159265358
2) Constant values specific to SOS_AEROSOLS		
SOS_MIE_DIM	Size of 2D arrays for the computation of Ricatti-Bessel functions (ψ_n , χ_n), derived functions (D_n and G_n) and coefficients A_n and B_n . (SOS_MIE)	10000 (for processing up to $\alpha_{\max} \approx 4990$)
SOS_MAXNB_ANG_EXT	Maximum size of 2D arrays for external phase functions (SOS_AEROSOLS)	200
SOS_MIE_ALPHAMIN	Minimum value of the Alpha size parameter in MIE's calculus. Must lie between 0,0001 and 10. Note : Must be given in double precision (SOS_AEROSOLS)	0.0001D+00
SOS_ALPHAMAX_WMO_DL	Maximum value of the size parameter for the MIE's computations of the WMO Dust-like component. (SOS_AEROSOLS)	4000
SOS_ALPHAMAX_WMO_WS	Idem for the WMO « Water Soluble » component.	50
SOS_ALPHAMAX_WMO_OC	Idem for the WMO « Oceanic » component.	800
SOS_ALPHAMAX_WMO_SO	Idem for the WMO « Soot » component.	10
SOS_ALPHAMAX_SF_SR	Idem for the Shettle & Fenn « Small Rural » component.	70
SOS_ALPHAMAX_SF_SU	Idem for the Shettle & Fenn « Small Urban » component.	90
SOS_COEF_NRMAX	Minimum value of the size distribution ratio $n(r) / N_{\max}$ for the determination of the maximum size parameter for Mie's computations. (SOS_AEROSOLS)	0.0001
SOS_AER_DATAWMO	File name for WMO data including the modal radius, the log of the variance, the volumetric concentration and the values of the refractive indices (real and imaginary part) as a function of the wavelength. File location : \$RACINE/fic (SOS_AEROSOLS)	Data_WMO
SOS_AER_DATASF	File name of Shettle & Fenn data including the log of the variance and the values of the modal radius as a function of the relative humidity. File location : \$RACINE/fic (SOS_AEROSOLS)	Data_SF
SOS_AER_SR_SF	File name of « Small Rural » data from Shettle & Fenn including refractive indices (real & imaginary part) as a function of the wavelength and the relative humidity. File location : \$RACINE/fic (SOS_AEROSOLS)	IRefrac_SR
SOS_AER_LR_SF	Idem for the « Large Rural » data from Shettle & Fenn.	IRefrac_LR
SOS_AER_SU_SF	Idem for the « Small Urban » data from Shettle & Fenn.	IRefrac_SU

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SOS_AER_LU_SF	Idem for the « Large Urban » data from Shettle & Fenn.	IRefrac_LU
SOS_AER_OM_SF	Idem for the « Oceanic model » data from Shettle & Fenn.	IRefrac_OM
SOS_PH_SEUIL_TRONCA	Threshold value for the truncation coefficient (SOS_AEROSOLS)	0.1
3) Constant values specific to the definition of an atmospheric profile		
SOS_OS_NT	Number of atmospheric profile layers (SOS_PROFIL, SOS, SOS_OS)	26
SOS_PROFIL_MIN_NBC	Minimum number of molecular sub-layers for a profile with variable positioning of aerosols between 2 altitudes. (SOS_PROFIL)	3
SOS_DZTRANSI	Definition of the thickness of the transition layer (km). (SOS_PROFIL)	0.010
4) Constant values specific to the computation of surface reflection matrices		
SOS_PH_TEST	Factor for the comparison of Gmin and Gmax. (SOS_GLITTER)	10000
SOS_PH_NU	Number of azimuthal angles ($2^{\text{SOS_PH_NQ}}$) (SOS_GLITTER, SOS_ROUJEAN, SOS_NADAL)	1024
SOS_PH_NQ	Power of 2 for SOS_PH_NU. (SOS_GLITTER)	10
SOS_SEUIL_SF_NADAL	Threshold value for stopping the expansion in Fourier series of the function (F21 Nadal) / (F21 Fresnel). (SOS_NADAL)	0.001
SOS_SEUIL_SF_ROUJEAN	Threshold value for stopping the expansion in Fourier series of Roujean's BRDF. (SOS_ROUJEAN)	0.001
SOS_TETAS_LIM_ROUJEAN	Maximum solar zenith angle for computing Roujean's BRDF (degrees). (SOS_ROUJEAN, SOS_NOM_FIC_SURFACE)	60
SOS_TETAV_LIM_ROUJEAN	Maximum viewing zenith angle for computing Roujean's BRDF (degrees). (SOS_ROUJEAN, SOS_NOM_FIC_SURFACE)	60
5) Constant values specific to the SOS program		
SOS_OS_IBOR	Minimal order of the expansion in Fourier series (SOS_OS)	0
SOS_PH_SEUIL_CV_SG	Convergence threshold of the geometric series (SOS_OS)	0.01
SOS_PH_SEUIL_SUMDIF	Multiple scattering threshold for the loop ending condition (SOS_OS)	0.00001
SOS_PH_SEUIL_SF	Threshold for the ending condition of the Fourier series expansion (SOS_OS)	0.0001
SOS_SEUIL_Z	Threshold value for computing the rotation angles (SOS_TRPHI)	0.0001
SOS_SEUIL_X	Threshold value for computing the terms M21 and M31 of the reflection matrix expressed in a frame tied to the meridian plane. (SOS_TRPHI)	0.00001

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6) Constant values specific to the definition of angles and orders of expansion		
6.1) Constant values related to the size of the 2-D arrays and to the maximum orders of expansion in Fourier series or Legendre polynomials.		
SOS_MIE_NBMU_MAX	Maximum number of angles (> 0) for dimensioning the 2D arrays used for the phase functions. Minimum value : number of Gauss angles by default + maximum number of user angles : SOS_DEFAULT_NBMU_MIE + SOS_NBMAX_USER_ANGLES. Do not define a value artificially too large : larger is the value, slower is the algorithm. (SOS_ANGLES, SOS_AEROSOLS, SOS_MIE)	100
SOS_OS_NBMU_MAX	Maximum number of angles (> 0) for dimensioning the 2D arrays used for the radiance field and surface reflection. Minimum value : number of Gauss angles by default + maximum number of user angles : SOS_DEFAULT_NBMU_LUM + SOS_NBMAX_USER_ANGLES. Do not define a value artificially too large : larger is the value, slower is the algorithm. (SOS_ANGLES, SOS_SURFACE, SOS_GLITTER, SOS_ROUJEAN, SOS_RONDEAUX_BREON, SOS_NADAL, SOS, SOS_OS, SOS_TRPHI)	68
SOS_OS_NB_MAX	Maximum order of expansion of the phase functions in Legendre polynomials and of expansions in Fourier series, used for dimensioning the 2D-arrays. Use $SOS_OS_NB_MAX \geq 2 \times SOS_MIE_NBMU_MAX$ (SOS, SOS_OS, SOS_AEROSOLS, SOS_SURFACE, SOS_ROUJEAN, SOS_NADAL)	200
SOS_OS_NS_MAX	Maximum order of expansion in Legendre polynomials of the Fresnel matrix terms for dimensioning the 2D-arrays. Use $SOS_OS_NS_MAX = 2 \times SOS_OS_NBMU_MAX$ (SOS_SURFACE)	136
SOS_OS_NM_MAX	Maximum order of expansion in Fourier series of the G function - weighting factor of the Fresnel matrix - for dimensioning the 2D-arrays. Use $SOS_OS_NM_MAX = SOS_OS_NB_MAX + SOS_OS_NS_MAX$ (SOS_SURFACE, SOS_GLITTER, SOS_RONDEAUX_BREON)	336

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6.2) Number of angles and maximum orders to use in case of no user-defined angles		
SOS_DEFAULT_NBMU_MIE	Default number of Gauss angles (> 0) for computing the aerosol radiative properties. (SOS_ANGLES)	40
SOS_DEFAULT_NBMU_LUM	Default number of Gauss angles (> 0) for the radiance field. (SOS_ANGLES)	24
SOS_DEFAULT_OS_NB	Default value of the maximum order of expansion of the phase functions in Legendre polynomials and of the radiance field in Fourier series. Use $SOS_DEFAULT_OS_NB \geq 2 \times SOS_DEFAULT_NBMU_MIE$ (SOS_ANGLES)	80
SOS_DEFAULT_OS_NS	Default value of the maximum order of expansion of the Fresnel matrix elements in Legendre polynomials. Use $SOS_DEFAULT_OS_NS = 2 \times SOS_DEFAULT_NBMU_LUM$ (SOS_ANGLES)	48
SOS_DEFAULT_OS_NM	Maximum order of expansion in Fourier series of the G function - weighting factor of the Fresnel matrix - for dimensioning the 2D-arrays. Use $SOS_DEFAULT_OS_NM \geq SOS_DEFAULT_OS_NB + SOS_DEFAULT_OS_NS$ (SOS_ANGLES)	128
6.3) Maximum number of angles for the files describing the angles to be used		
SOS_NBMAX_USER_ANGLES	Maximum number of user-defined angles, in addition to the Gauss angles (SOS_ANGLES)	20
SOS_NBANGLES_MAX	Maximum number of positive angles (Gauss angles + user-defined angles + 1 = solar zenith angle). Must be the maximum of SOS_MIE_NBMU_MAX and SOS_OS_NBMU_MAX (SOS_ANGLES)	100
SOS_SEUIL_ECART_MUS	Difference threshold between cos(X) and cos(θ_s) under which $\theta_s = X$ (numerical error allowed) (SOS_ANGLES)	0.00001

III-3.2 Modification of the number of profile layers

In order to refine the optical thickness profile (for example, in the case of a dense atmosphere), the number of layers may be increased. Since this parameter affects the size of the 2D-arrays, the number of profile layer is defined in the file SOS.h by the constant value SOS_OS_NT. The user may change its value. Note that it is necessary to recompile in order to take into account the new value.

IV- Software description

This section summarizes the software architecture. A complete description of the programs and methods is available in the following chapters

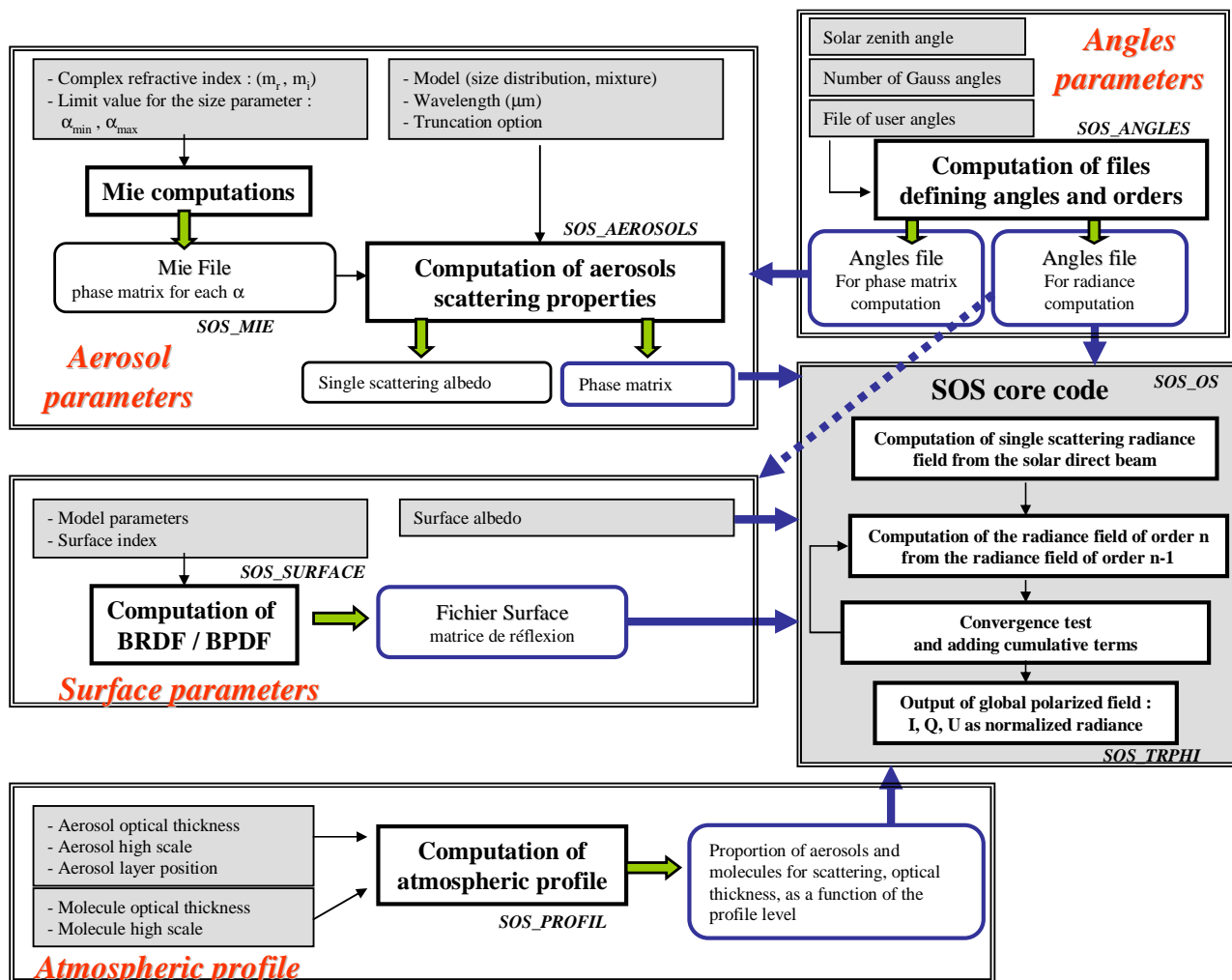


Figure 7 : High level view of the processing steps managed by the shellscript `main_SOS`.

The code is divided in 5 processing blocs :

- Preparation of angles to be used and maximum orders of expansion.
- Computation of the surface reflection matrix for a simulation over the sea (determination of sunglint) or over land surfaces (BRDF and BPDF).
- Processing of the aerosol scattering properties : Mie calculations as a function of the chemical nature of particle (refractive index) and determination of the phase matrix for a given model and wavelength.

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- Computation of the atmospheric profile as a function of the total optical thickness of molecules and aerosols: relative contribution to scattering for the aerosols and for the molecules as a function of the profile level, total optical thickness of the mixture as a function of the level.
- Processing of successive atmospheric scattering effects and surface/atmosphere reflections.

The main script main_SOS.ksh is in charge of the workflow and calls to the different functions.

In the case of the simulation of the radiance for a wavelength λ_{simu} with the aerosol optical thickness defined for λ_{ref} the script computes the cross-section of aerosol extinction for the two wavelengths so as to estimate the optical depth for λ_{simu} .

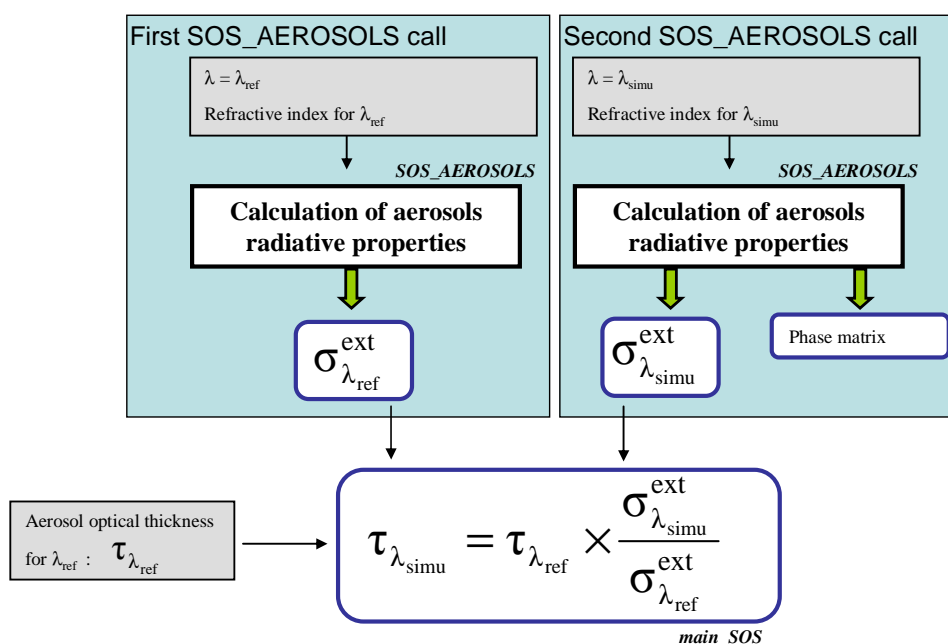


Figure 8 : Estimates of the aerosol optical thickness at the radiance field wavelength.