User's Guide for the

Software Package SCIATRAN

(Radiative Transfer Model and Retrieval Algorithm)

- Version 3.8 -

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Contents

1 Introduction

1.1 General

This user's guide describes how SCIATRAN 3.8 software package can be installed and run on a LINUX PC. The described procedure is expected to be nearly the same for any other computer running UNIX/LINUX. The program is also reported to work under Microsoft WINDOWS. However, we can not offer any installation/execution support for WINDOWS users.

SCIATRAN 3.8 is a software package incorporating a radiative transfer model and a retrieval algorithms which can be adapted to solve a wide range of scientific tasks. The program has been developed at the Institute of Environmental Physics/Institute of Remote Sensing (IUP/IFE), University of Bremen, Germany.

SCIATRAN 3.8 has been written in FORTRAN 2003. The main target computer platform is Intel/AMD PC under LINUX operating system. At this platform, the program is configured to work with ifort ($\geq$ 2011) and gfortran ($\geq$ 4.9) compilers. Although other computer platforms/compilers can also be used, this might require an appropriate adaptation of the system environment and Makefile. Due to technical reasons we are not able to provide any support for platforms/compilers other than listed above. Please also be advised that ***I*UP/IFE cannot make any warranties that the program is free of errors**. Users are encouraged to send bug reports to SCIATRAN support team (contact address can be found in SCIATRAN web page $h$ttp://www.iup.physik.uni-bremen.de/sciatran).

The radiative transfer model incorporated into the SCIATRAN 3.8 software package has been designed to perform fast and accurate simulations of radiance spectra appropriate to atmospheric remote sensing observations in the UV-visible-TIR spectral range (limited capability in MWIR-TIR) in either vector or scalar mode. In addition, a coupled ocean-atmosphere system can be considered to simulate the radiance over and under the water surface (in scalar mode). The radiative transfer model is linearized with respect to a variety of atmospheric parameters, i.e., appropriate weighting functions can be obtained in any supported observation mode.

During the last years several papers have been published and diploma and PhD theses generated demonstrating that SCIATRAN is a valuable tool suitable for a wide range of applications, see e.g. Rozanov et al. (2000, 2001); Rozanov (2003); Postylyakov et al. (2001); Mueller et al. (2002); Wittrock et al. (2004); Bruns et al. (2004); Loughman et al. (2004); Kokhanovsky et al. (2004); von Savigny et al. (2005b); Rozanov et al. (2005); **?**); **?**); **?**); **?**, 2007); **?**); **?**); **?**); **?**. Among others these are the retrieval of atmospheric constituents from measurements of direct or scattered solar light, calculation of air mass factors and slant columns of atmospheric trace gases, and the retrieval of aerosol and cloud parameters. Many

of these papers also contain comparisons with other models or measurements. Therefore, we consider this model to be sufficiently validated. Nevertheless, validation is a never ending and still ongoing task. It is especially important when applying the program to "new" areas or after program modification.

1.2 Features overview

Highlights:

Polarized (vector) radiative transfer, spherical atmosphere, coupled ocean-atmosphere system, rotational Raman scattering in the atmosphere (including electron spin-rotational splitting), vibrational Raman scattering and Colored Dissolved Organic Matter (CDOM) fluorescence in the ocean, photochemically active species.

Products:

Modeling:
radiance/intensity (scalar mode) or Stokes vector (vector mode), weighting functions for scalar and vector case (limited capability in vector case), air mass factors (AMF), slant columns, vertically resolved AMFs (box AMFs), fluxes (actinic, upwelling, downwelling, diffuse and total), spherical albedo, diffuse transmission, vertical optical depth.
Retrieval (not included in a freely distribute package):
trace gas vertical profiles and total columns, aerosol extinction coefficient, cloud parameters (top height, optical thickness, liquid water content, effective radius of water droplets), surface albedo, height of the effective Lambertian reflecting surface, tangent height correction.

Wavelength range:

In general, the radiative transfer calculations can be done from 175.44 nm to 40 microns. Several spectral windows can be selected. It should be noted, however, that in certain spectral intervals the program capabilities are limited. In MWIR-TIR spectral range one should be aware that only an equilibrium thermal emission (Planck distribution) and no gaseous emission structure is accounted for. The correlated-k approach (ESFT mode) can be used only in the spectral intervals related to GOME/SCIAMACHY spectral channels (240–1750 nm, 1940–2040 nm, and 2260–2385 nm), and selected spectral interval for wavelength larger than 3000 nm see Sec. 3.10.4 for details.

Geometry:

The radiative transfer calculations can be done for any observation geometry as well as any location of the instrument (in the space, on the ground, within the atmosphere or under a water surface). However, for some observation modes the program features are limited.

Atmospheric model:

Trace gases (O_3, NO_2, ClO, OClO, BrO, HCHO, SO_2, NO_3, O_4, O_2, H_2O, CO_2, CO, CH_4, N_2O, NO, NH_3, HNO_3, OH, HF, HCL, HBR, HI, Na, Mg, Mg^+), Rayleigh scattering, aerosols, clouds.

Underlying surface reflection:

Lambertian reflection with wavelength dependent or constant albedo. Bidirectional reflectance distribution function (BRDF) including parameterizations for a variety of surface types (not in all program modes). A surface elevation with respect to the sea level can be specified.

Additional features for water surface reflection:

Fresnel reflection from absolutely calm and wind-roughed ocean surface (accounting for polarization), whitecap reflection, water leaving radiation.

Underwater radiative transfer:

Absorption by pure water, chlorophyll, and CDOM. Scattering by pure seawater and particulate matter.

New features in SCIATRAN 3.8:

- Weighting functions for the main parameters of PROSAIL model are included to provide linearized radiative transfer calculations within the canopy.
- Database of optical parameters of ice clouds was extended and includes now the "Ice cloud bulk single-scattering property spectral models from the UV through the Far-infrared" from B.A. Baum.
- The rotational Raman scattering in atmosphere can be calculated now accounting for polarization in plane-parallel and spherical atmosphere.

Open issues:

- Non-LTE emission structures such as the NO-γ emission band around 260 nm or the $O_2(a^1\Delta_g)$ emission band around 1.27 nm are not implemented.
- Pressure dependence of all absorption cross-sections (except for those of line-absorbers) is not accounted for.
- Weighting functions are not yet implemented for a coupled ocean-atmosphere system.
- Vector mode is not yet available for a coupled ocean-atmosphere system.

2 Quick Start

2.1 Supported computer systems

- Intel/AMD PC under LINUX operating system with gfortran ($\geq$ 4.9) or Intel Fortran Composer ($\geq$ 2011). For these computer systems full installation, running and debugging support is provided.
- Any other LINUX/UNUX system with any other FORTRAN 2003 compiler (an appropriate adaptation of the system environment and Makefile by user might be necessary). For these computer systems/compiles only a limited installation, running and debugging support can be offered.
- SCIATRAN is also reported to work under Microsoft WINDOWS. Unfortunately, we cannot offer any instalation or execution support for WINDOWS users.

2.2 Software requirements

- FORTRAN 2003 Compiler: Intel Fortran Composer ($\geq$ 2011) or gfortran ($\geq$ 4.9) are recomended.
- LAPACK and BLAS FORTRAN libraries (http://netlib.org/lapack)
- Optionally (retrieval mode only): GALAHAD Quadratic Programming Library (double precision version). The library is needed for some retrieval modes only, see Sec. 4.9 and 4.14 for details.
  (http://galahad.rl.ac.uk/galahad-www/download.html)

2.3 How to install the LAPACK and BLAS Libraries

- Go to the http://netlib.org/lapack web page and scroll down for download area.
- Dowload the "lapack.tgz" file containing the most recent LAPACK/BLAS libraries.
- Type "tar -zxpf lapack.tgz" to unpack the libraries. This will create a subdirectory named "lapack-X.X.X", where "X.X.X" denotes the version number of the LAPACK/BLAS libraries, e.g., "lapack-3.6.0".
- Type "cd lapack-X.X.X" to change to this directory ("X.X.X" has to be replaced by the actual version number).

- Look in the subdirectory “INSTALL” for a “make.inc” file which corresponds to your compiler, e.g., “make.inc.ifort” for Intel Fortran Composer (ifort).
- Copy this file into “make.inc” and put it into the main LAPACK directory, e.g., “me@computer:∼/lapack-3.6.0¿ cp INSTALL/make.inc.ifort make.inc”
- If no appropriate “make.inc” file is available, edit “make.inc.example” file in the main LAPACK directory adjusting the compiler name and options as needed.
- Compile BLAS libraries typing “make blaslib”
- Compile LAPACK libraries typing “make lapacklib”
- Put the compiled library files into “/usr/lib” directory (root privileges are needed) as follows:
  - If you intend to use only one compiler at your computer:
    cp librefblas.a /usr/lib/libblas.a
    cp liblapack.a /usr/lib/liblapack.a
  - If you intend to use multiple compilers at your computer:
    cp librefblas.a /usr/lib/libblas_{COMPILER_NAME}.a
    cp liblapack.a /usr/lib/liblapack_{COMPILER_NAME}.a
    where, e.g. for Intel Fortran Composer, “ifort” has to be substituted instead of “{COMPILER_NAME}”.
  - Please note that for newer versions of lapack distributions the library file libref-blas.a is generated instead of libblas.a as it was before. For compatibility reasons the library is renamed in accordance with the old convention.

2.4 System environment

For a successful compilation and execution of the program some system/shell environment variables must be set. In this section the bash syntax is used. For other shells the commands need to be adapted properly. If you want to make the settings permanent put the commands listed below into the “.bashrc” or “.profile” file in your home directory.

- Check if the “$HOSTTYPE” system variable is set properly. To do this type “echo $HOSTTYPE”. Typical settings are “x86_64” for modern 64 bit PCs and “i586” for older 32 bit computers. If the variable is empty we recommend to set it accordingly to your computer platform type, e.g., “export HOSTTYPE=x86_64” (this is the command to put in, e.g., “.bashrc” file). This setting is, however, not mandatory. If this variable is left empty, the object directories and executable files will be labeled with “unknown” (not crucial for program compilation and execution).
- Unlimit the stacksize typing “ulimit -s unlimited” (this is the command to put in, e.g., “.bashrc” file). This setting is crucial for a successful program execution.

2.5 How to install the GALAHAD Quadratic Programming Library

You can skip this section if you do not want to install the GALAHAD Quadratic Programming library (needed for some retrieval modes only, see Sec. 4.9 and 4.14).

- Go to the http://galahad.rl.ac.uk/galahad-www/registration.html web page and fill out the registration form to get the access to the GALAHAD library.
- Go to http://galahad.rl.ac.uk/galahad-www/downloads/download.html, input your login data, and then download the library sources ("galahad.tar.gz" file).
- Store the library sources in any directory you want and type "gunzip galahad.tar.gz" to unpack the library.
- Type "tar xvpf galahad.tar" to untar the library. This command will create your a subdirectory named "galahad" containing the library files.
- At this point you can either perform a standard installation of the double precision library following the instructions listed in the "galahad/README" file (skip the rest of this section in this case) or follow the instruction below for a partial installation.

Keep reading only if you chose the partial installation. Otherwise skip the rest of this section.

- Create (or download) the "copy_for_sciatran.sh" shell script, as described in Sec. A.2, in(to) the "galahad" directory and start it in the "bash" environment supplying the name of the directory where the GALAHARD files needed for SCIATRAN will be placed to, e.g., "bash copy_for_sciatran.sh *YOUR_GALAHARD_DIR*". A subdirectory "SRC" will be created in the specified directory where all source files from the GALAHAD library, which are needed to run SCIATRAN, will be copied to. If you can not use the shell script just copy all files listed in Sec. A.1 ("needed_for_sciatran.txt" file) into the "*YOUR_GALAHARD_DIR*/SRC" directory.
- Go to the http://hsl.rl.ac.uk/archive/hslarchive.html and fill out the registration form to get access to the HSL archive.
- Download the "MA27" package from the HSL archive web site (http://hsl.rl.ac.uk/archive/hslarchive/packages/packages.html) and put it as "ma27.f" file into the "*YOUR_GALAHARD_DIR*/SRC" directory.
- Change to the "*YOUR_GALAHARD_DIR*" directory.
- Create (or download) the Makefile as described in Sec. A.3. The current version of the Makefile supports Intel Fortran Composer (ifort), gfortran, g95, and xlf (IBM) compilers. For use with other compilers the Makefile needs to be appropriately adapted.
- Type "gmake fc={COMPILER_NAME}" to compile the library. Here the "{COMPILER_NAME}" can be one of "ifort", "gfortran", "g95", or "xlf95_r". This command will create a library file named "libgalahad.a" as well as several module files ("*.mod") which will be placed into the "OBJ_{HOSTTYPE}_{COMPILER NAME}" subdirectory (the subdirectory is created automatically). Here, "{HOSTTYPE}" is retrieved from the corresponding system environment variable (see Sec. 2.4 for details).

If you can not use Makefile, create the library and module files manually compiling the source files in the order listed in Sec. A.1 ("needed_for_sciatran.txt" file).

2.6 How to install SCIATRAN

- Download SCIATRAN 3.8 (sciatran-3.8.X.tgz), SCIATRAN Data Base (data_bases.tgz), and SCIATRAN local data (local_data.tgz) from the SCIATRAN web page (http://www.iup.physik.uni-bremen.de/sciatran).
- Unpack SCIATRAN Data Base (data_bases.tgz) wherever you want as follows:
  - type "gunzip data_bases.tgz", file data_bases.tar will be created;
  - type "tar xvpf data_bases.tar", a subdirectory DATA_BASES will be created;
  - remove data_bases.tar file.
- Create directory "SCIATRAN" and change to this directory.
- Move both remaining *.tgz files into the current directory.
- Unpack SCIATRAN 3.8 (sciatran-3.8.X.tgz):
  - type "sciatran-3.8.X.tgz", file sciatran-3.8.X.tar will be created;
  - type "tar xvpf sciatran-3.8.X.tar", a subdirectory Execute-3.8 will be created;
  - remove sciatran-3.8.X.tar file.
- Unpack SCIATRAN local data (local_data.tgz):
  - type "local_data.tgz", file local_data.tar will be created;
  - type "tar xvpf local_data.tgz", a subdirectory data will be created;
  - remove sciatran-3.8.X.tar file.
- Change to Execute-3.8 subdirectory.
- Create subdirectories "OBJ_{COMPUTER SYSTEM}" and "OBJ_{COMPUTER SYSTEM}_DBG". Pre-defined values for "{COMPUTER SYSTEM}" are "ALPHA" for COMPAQ Alpha, "SUN" for SUN, "INTEL" for PC under Linux using Intel "ifort" Compiler, "IBM" for IBM Regatta, i.e., for example, on a SUN workstation you have to type mkdir OBJ_SUN and mkdir OBJ_SUN_DBG to get a required directory structure.
- If you obtain the full SCIATRAN distribution (including retrieval module) and do not want to install the GALAHAD Quadratic Programming library (needed for some retrieval modes only, see Sec. 4.9 and 4.14), copy "shi_squ_dummy.f" to "shi_squ.f" and "iterate_no_galahad.f" to "iterate.f". Otherwise, adjust the paths to the GALAHAD library and the GALAHAD modules in the Makefile, e.g., for "ifort" compiler:
  FFLAGS = -O3 -module $(OBJDIR) -I *YOUR_GALAHARD_DIR*/OBJ_IFORT -u -w95
  LNFLAGS = $(FFLAGS) -L *YOUR_GALAHARD_DIR*/OBJ_IFORT -lgalahad -llapack_ifort -lblas_ifort

For the standard distribution (radiative trnsfer model only) this is already done by default and you do not need to change anything.

- Compile the program typing "gmake" for optimized version and "gmake debug=true" for debugger version.

2.7 Control files

In SCIATRAN there is four levels of control input files. Main control files are shown in Fig. 2.1. The level 1 (main level) consists of two files only. They are:

- control.inp - main control file;
- control_geom.inp - geometry of observation and illumination settings.

It should be pointed out that user must look in these two files only for the first run.

The second level of control files (shown by green color in Fig. 2.1) consist of four following inputs files:

- control_ray.inp - Rayleigh scattering advanced settings.
- control_prof.inp - temperature, pressure, and gaseous absorber profiles advanced settings;
- control_ac.inp - advanced settings related to the accuracy and speed of the radiative transfer calculations;
- control_out.inp - output format advanced settings.

For the first run of SCIATRAN user can used default mode to install all input parameters in these four control files.

Third level of control files (shown in Fig. 2.1 by hell-blue color) should be used to solve different practical problems of atmospheric, oceanic, and surface optics. The user needs to configurate these control files only if the corresponding option is switch on in the control.inp file. These input files are listed below:

- control_aer.inp - aerosol parameters;
- cloud.inp - cloud parameters;
- control_la.inp - gaseous line absorber parameters setup;
- xsection.inp - gaseous absorption cross-section setup;
- control_brdf.inp - parameters of surface BRDF;
- control_conv.inp - convolution with instrument response function;
- control_te.inp - thermal emission setup;
- control_pas.inp - photochemically active species setup;
- control_uwt.inp - ocean-atmosphere setup;
- control_ret.inp - retrieval setup;
- control_wf.inp - weighting function setup.

It follows that the third level consists of eleven control files. The large number of input files is due to the fact that SCIATRAN is a package capable to solve most of practical problems of atmospheric, oceanic, and surface optics (including, e.g., snow, ocean, and vegetation). We note, however, that as a rule, only few input files need to be changed (in subsequent runs), if the general setup is prepared.

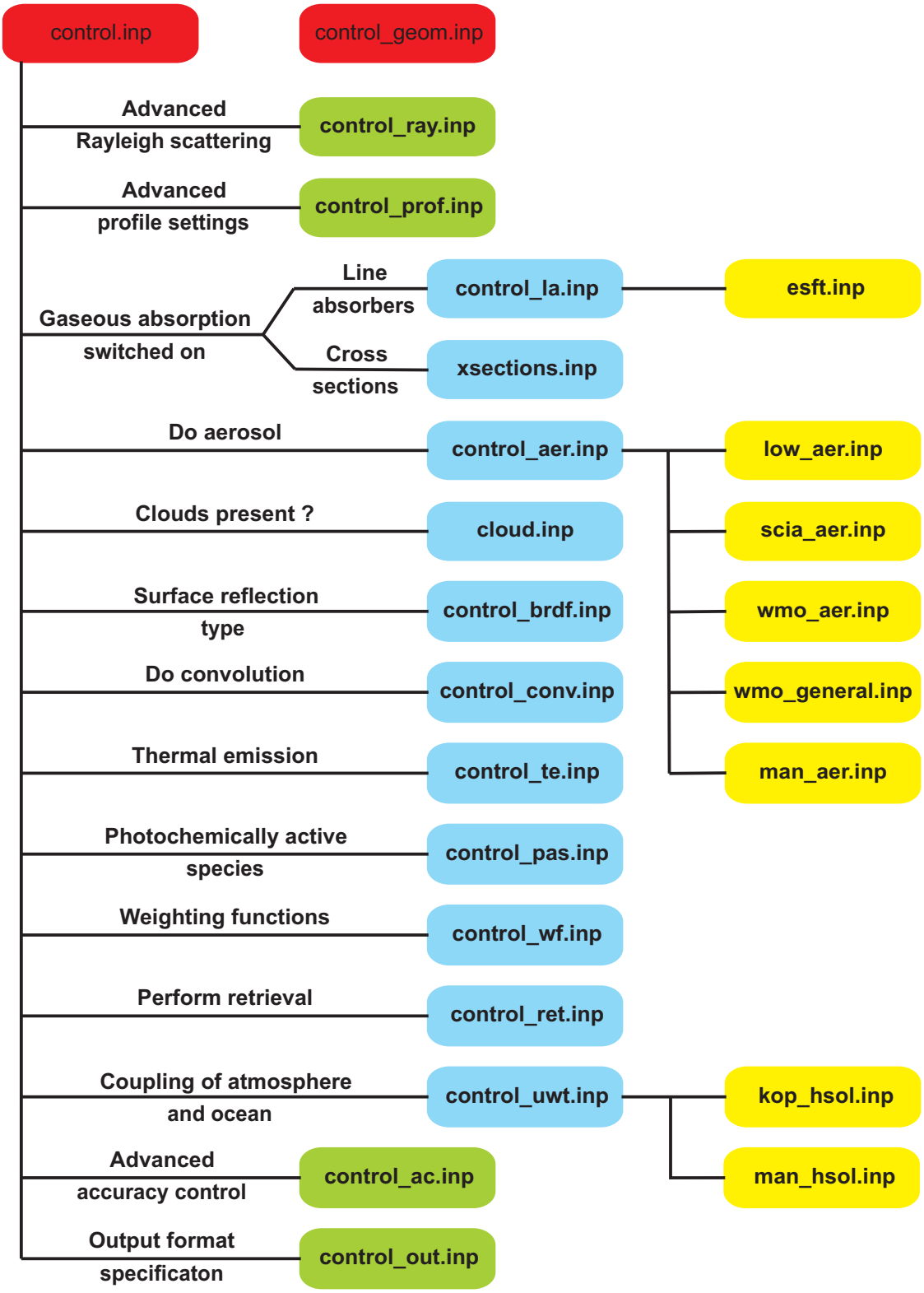

Figure 2.1: SCIATRAN contol files

The fourth level of input files should be used by the user to adjust the parameters needed for the solution of a specific forward or inverse radiative problem. These files are shown in Fig. 2.1 by yellow color and listed below:

- esft.inp - ESFT setup.
- low_aer.inp - LOWTRAN aerosol setup.
- scia_aer.inp - SCIATRAN database aerosol setup.
- wmo_aer.inp - WMO database aerosol settings.
- wmo_general.inp - WMO database aerosol setup.
- man_aer.inp - manual aerosol settings.
- mie_aer.inp - aerosol settings for Mie code.
- kop_hsol.inp - hydrosol scattering matrices settings.
- man_hsol.inp - manual hydrosol matrices settings.

The structure of these user interface files is as follows: All user input files contain:

- comment lines (lines beginning with "#"),
- empty lines,
- lines containing "keywords" (for example, "Aerosol settings"), which will be called control parameter or parameter,
- and subsequent lines of input settings (for example: "off").

Only those lines containing the input settings are to be modified by user.

All comment lines (i.e., lines beginning with "#") and all empty lines can be removed. It is sufficient to have sequences of one line containing the "keyword" followed by one line (or several lines if required) containing the user selected settings. In general it is even possible to change the order of "keywords" but not the sequence and sentence within "keywords".

All input files (with comments) are given in Appendix C.

2.8 How to check SCIATRAN (plane-parallel geometry)

Appropriate control file: "control.inp"
Relevant control parameters: "Home directory"

Before using the SCIATRAN package for solution of specific problem it is strongly recommended to check that the instalation of source code was successful. For this purpose we have prepared numerous tests based on the International Polarized Radiative Transfer (IPRT) inter-comparison project (see (Emde et al., 2015) for details).
To perform test calculations please follow the instructions:

- Set in the "Home directory" control line of the control.inp file the path to directory "SCIATRAN";
- Change directory to "IPRT_TEST";
- Start the shell-script file "all_tests.sh" as follows:
  "./all_tests.sh par1 par2 "
  where parameters "par1" and "par2" are the path to the directory "../Execute_3.8" and the name of appropriate executable "SCIA_{COMPUTER SYSTEM}.exe", respectively;

- The program performs calculation of test scenarios A2 - A6 and B1 - B4 which are described in (Emde et al., 2015).
  If the calculation of the corresponding test is finished successfully, on the screen user can see the following information

```
Perform test A4
---------------
   Comparison results of test A4 - Spheroidal aerosol particles:
   SCIATRAN    IPOL      PSTAR    V-3.5.9
I   0.0760    0.0880    0.0250    0.0760
Q   0.0284    0.0280    0.0280    0.0284
U   0.0342    0.0340    0.0350    0.0342
V   1.2772    1.2770    1.2780    1.2772
 ***** Comparison is successful *****
```

  Output results consist of five columns:
  - first column is the identification of the Stokes vector component;
  - second column contains comparison of the current SCIATRAN version and MYSTIC MC code;
  - third and fourth columns show results of IPOL and PSTAR codes comparisons with MYSTIC MC code as given in Table 3 (tests A2-A6) and Table 4 (tests B1-B4) by Emde et al. (2015);
  - fifth column contains results for SCIATRAN version v3.5.9, which is considered as reference.

  The `***** Comparison is successful *****` message is obtained if the maximal relative difference between current results and results for the 3.5.9 version is smaller than 0.1%.

Note that in order to quantify the level of agreement between the models we calculate the relative root mean square differences Δ between MYSTIC and other codes for the full radiation field including all up- and down-looking directions. This yields one representative number for each test case. We define Δ_I for I as follows:

$$\Delta_I = \sqrt{\frac{\sum_{i=1}^{N}(I^i_{MYSTIC} - I^i_m)^2}{\sum_{i=1}^{N}(I^i_{MYSTIC})^2}}\,. \tag{2.1}$$

Here m denotes the radiative transfer model and the summation is done over all N directions, for which the radiation field was calculated. For other Stokes components Δ is calculated accordingly.

Attention:

- Depending on the computer platform the calculation of all tests may take a few tens of minutes.
- Note that tests based on the IPRT inter-comparison project enable the plane-parallel approximation of the SCIATRAN code to be checked only. The user must be careful when using other options.

2.9 How to check SCIATRAN (spherical geometry)

Appropriate control file: "control.inp"
Relevant control parameters: "Home directory"

In the previous section we described how to check instalation of source code in the case of plane-parallel geometry. Here we suggest an additional tests to check the instalation of SCIATRAN in the case of spherical geometry. To do this we have pre-calculated Stokes vector components of the reflected and transmitted radiation at the top and bottom of atmosphere, respectively, at the wavelength 500 nm. The calculations were performed for zenith angles 10°, 20°, 30°, 40°, 50°, 60°, 70°, 80°, azimuthal angles 30°, 60°, 90°, and solar zenith angle was set to 50°. We have selected three scenario:
- Rayleigh atmosphere ("SPH_R"),
- Rayleigh and aerosol atmosphere ("SPH_RA"),
- Rayleigh and aeroso atmosphere including a water cloud ("SPH_RAC").
In addition to these scattering processes we included gaseous absorption by O_3 and NO_2 and reflection of radiation on the Lambertian surface with albedo 0.3. The results obtained using the SCIATRAN version 3.8.4 were saved and will be called throughout this section as reference.

To perform test calculations please follow the instructions:

- Set in the "Home directory" control line of the control.inp file the path to directory "SCIATRAN";
- Change directory to "SPHER_TEST";
- Start the shell-script file "all_tests.sh" as follows:
  "./all_tests.sh par1 par2 "
  where parameters "par1" and "par2" are the path to the directory containing executable, e.g., "../Execute_3.8" , and the name of appropriate executable "SCIA_{COMPUTER SYSTEM}.exe", respectively;
- The program performs calculation of test scenarios SPH_R, SPH_RA, and SPH_RAC. If the calculation of the corresponding test is finished successfully, on the screen user can see the following information (example is given for test SPH_RAC):

```
Perform test SPH-RAC
--------------------
  Comparison results of test SPH_RAC -
      Rayleigh, aerosol and cloud scattering above Lambertian surface
      Reference         Current     Rel.max   Rel.mean
I    0.3714554E-01    0.3714554E-01   0.0000   0.0000
Q    0.8862606E-04    0.8862606E-04   0.0000   0.0000
U    0.5032893E-04    0.5032893E-04   0.0000   0.0000
V    0.5493627E-06    0.5493627E-06   0.0000   0.0000
***** Comparison is successful *****
```

  Output results consist of five columns:
  - first column is the identification of the Stokes vector components;
  - second column contains minimal value of Stokes components for all viewing geometries of the reference SCIATRAN version;
  - third column contains minimal value of Stokes components for all viewing geometries

of the current SCIATRAN version;

- fourth column shows the relative difference in [%] between reference and current versions for these minimal values;
- fifth column contains the relative difference in [%] between reference and current versions calculated for all viewing geometries (N = 48).

The `***** Comparison is successful *****` message is obtained if the maximal relative difference between current and reference results is smaller than 0.1%.

Note that in order to quantify the level of agreement between the reference and current version we calculate the relative root mean square differences Δ between versions for the full radiation field including all up- and down-looking directions. This yields one representative number for each test case. We define Δ_I for I as follows:

$$\Delta_I = \sqrt{\frac{\sum_{i=1}^{N}(I_r^i - I_c^i)^2}{\sum_{i=1}^{N}(I_r^i)^2}}\,. \tag{2.2}$$

Here subscripts r and c denote reference and current version, respectively, and the summation is done over all $N = 48$ directions, for which the radiation field was calculated. For other Stokes components Δ is calculated accordingly.

Attention:

- Depending on the computer platform the calculation of all tests may take a few tens of minutes.

3 Radiative transfer modeling with SCIATRAN

3.1 What do you intend to calculate?

Appropriate control file: "control.inp"
Relevant control parameters: "RTM Mode"

Using the "RTM Mode" control parameter, user can switch between 11 major program modes depending on what is intended to be calculated:

- "int" - intensity or Stokes vector at boundaries or within the medium (Sec. 3.1.1);
- "flux" - fluxes at boundaries or within the medium (Sec. 3.1.2);
- "spher_alb" - spherical albedo and diffuse transmission (Sec. 3.1.3);
- "vod" - the vertical optical thickness of atmospheric trace gases, Rayleigh, aerosol, and cloud scattering and absorption (Sec. 3.1.5);
- "amf", "slant_col", "block_amf" - air mass factors, slant columns, or height resolved air mass factors (Sec. 3.1.4);
- "raman" - intensity or Stokes vector at boundaries or within the medium accounting for the rotation Raman scattering (Sec. 3.1.7);
- "wf" - weighting functions for atmospheric and surface parameters (Sec. 3.1.6);
- "num_pert" - numerical perturbation technique to check selected weighting functions (Sec. 3.1.8);
- "ret" - retrieval of atmospheric and surface parameters (Sec. 3.1.9).

The program modes available in SCIATRAN 3.8 are described in details below.

3.1.1 Intensity/Stokes vector ("int")

Relevant control parameters: "RTM Mode", ' 'Extra-terrestrial solar flux", "RTM-CORE"

Setting "RTM Mode" parameter to "int", the intensity or the Stokes vector (in the vector mode) of radiation field is calculated. The output units depend on the the setting of "Extra-terrestrial solar flux" parameter (see Section 3.2).

3.1.2 Fluxes ("flux")

Relevant control parameters: "RTM Mode", "RTM_TYPE", "Extra-terrestrial solar flux", "Lower and upper boundary of flux results"

Setting "RTM Mode" parameter to "flux" the following fluxes at each altitude level are calculated:

- actinic flux ;
- upwelling and downwelling diffuse fluxes ;
- upwelling diffuse scalar flux ;
- upwelling and downwelling total fluxes;
- direct solar radiance.

The output units are controlled by "Extra-terrestrial solar flux" parameter (see Section 3.2). The fluxes and the direct solar radiance are calculated at all altitude levels defined by the main altitude grid (see Section 3.3) and all solar zenith angles specified in "Solar zenith angles" control line (see Section 3.8.1) and written out in the altitude region as specified by "Lower and upper boundary of flux results" parameter (lower and upper altitude in km must be specified in the "control_out.inp" input file).
Attention:

- Settings of other geometrical parameters discussed in Section 3.8, such as viewing and azimuth angles as well as user defined output altitude, have no effect.
- If "Extra-terrestrial solar flux" parameter is set to "t", solar irradiance is written out as well.

Limitation:

- No fluxes can be calculated in solar/lunar occultation mode (parameter "RTM_TYPE" set to "transmission") .

3.1.3 Spherical albedo, diffuse transmission ("spher_alb")

Relevant control parameters: "Lower and upper boundary of flux results", "RTM Mode", "RTM_TYPE", "RTM-CORE" .

Setting "RTM Mode" parameter to "spher_alb" the spherical albedo and diffuse transmission are calculated.
The spherical albedo and diffuse transmission are calculated at all altitude levels defined by the main altitude grid (see Section 3.3) and written out in the altitude region as specified by "Lower and upper boundary of flux results" parameter (lower and upper altitude in km must be specified in the "control_out.inp" input file).
Attention:

- The only relevant parameter for this mode (except of the wavelength range) is the number of solar zenith angles which is used by the program to perform integration of the intensity over the solar zenith angles. The choice of the solar zenith angles grid is done automatically (Gaussian nodes) but the number of angles should be defined by the user (see "Solar zenith angles" control parameter in the "control_geom.inp" input file).
  Settings of other geometrical parameters discussed in Section 3.8, such as solar zenith angles, viewing and azimuth angles as well as user defined output altitude, have no effect.

Limitation:

- the spherical albedo and diffuse transmission can only be calculated for a plane-parallel atmosphere ("RTM_TYPE" control parameter is set to "pp_scat") in the discrete ordinate mode ("RTM-CORE" control parameter is set to "DOM_S" or "DOM_V").

3.1.4 Air mass factors/Slant columns/Block air mass factors ("amf"/"slant_col"/"block_amf")

Relevant control parameters: "RTM Mode", "Trace gas selection - AMF calculation".

Setting "RTM Mode" parameter to "amf", "slant_col" or "block_amf" air mass factors, slant columns, or height resolved air mass factors (so-called block air mass factors), respectively, are calculated. The parameter "Trace gas selection - AMF calculation" defines an atmospheric trace gas which calculations will be done for. Additionally, in "amf" and "slant_col" modes, local vertical columns (potentially solar zenith angle dependent, see Section 3.12.2.5) for the selected gas are calculated.
Limitation:

- Only single absorber can be selected employing "amf"/"slant_col"/"block_amf" mode.

3.1.5 Vertical optical depth ("vod")

Relevant control parameters: "RTM Mode", "RTM_TYPE", "RTM-CORE", "Forward model: trace gases"

Setting "RTM Mode" control parameter to "vod" the vertical optical depth for atmospheric trace gases selected in "Forward model: trace gases" (see Section 3.10) are calculated. If "RTM-CORE" is set to "DOM_S" or "DOM_V" (see Section 3.6), the vertical optical depths for Rayleigh scattering, aerosol scattering and absorption, cloud scattering and absorption, as well as total optical depth are calculated additionally.
Limitation:

- Vertical optical depths can not be calculated in solar/lunar occultation mode (parameter "RTM_TYPE" set to "transmission") .

3.1.6 Weighting functions ("wf")

Appropriate control files: "control.inp", "control_wf.inp"
Relevant control parameters: "Absolute or relative WF", "Extra-terrestrial solar flux", "Ocean parameters - weighting functions", "RTM Mode", "RTM_TYPE", "RTM-CORE", "Weighting functions: aerosol parameters", "Weighting functions for Stokes component", "Weighting functions: trace gases", "Weighting functions: other atmopsheric parameters", "WF normalization",

Setting "RTM Mode" parameter to "wf", weighting functions and intensity or Stokes vector are calculated. Under weighting function we understand the partial derivative of the intensity or components of the Stokes vector with respect to the corresponding parameter which is often called as Jacobian also. The intensity output is controlled in the same way as in "int" mode. Similar to the intensity, the output units for weighting functions depend on the setting of "Extra-terrestrial solar flux" parameter (see Section 3.2).
Parameters which the weighing function will be calculated for are selected in the "control_wf.inp" input file. In this file user can select the following options relevant to the weighting function calculations.

- Selection of Stokes components.
  Setting appropriate flags in
  ```
  # I  Q  U  V
  ```
  "Weighting functions for Stokes component"
  ```
    t  t  t  f
  ```
  control line to "t", the weighting function for all or for desired components of the Stokes vector can be calculated. The above setting forces the program to calculate weighting functions for I, Q, and U components of the Stokes vector with respect to the atmospheric or surface parameters selected below.
  Attention:
  - The calculation of the weighting function for the Stokes vector components is implemented for selected modes only.

- Trace gas weighting function selection.
  The weighting functions for atmospheric trace gases can be selected using the input field of the "Weighting functions: trace gases" parameter. The weighting functions can be used either in the relative or in the absolute representation. The relative weighting functions are multiplied by the vertical profile of the corresponding atmospheric parameters and related to relative variations of these parameters whereas absolute weighting functions are related to absolute variations of the parameters.

  Each input line contains one or multiple control sequences separated by a semi-colon. Each control sequence contains at the beginning 'A' or 'R' character to select between the absolute or relative weigthing functions, respectively, separated by a colon from the parameter list. The latter contains comma or space separated list of parameter names or 'all' to select all available weighting functions. Using 'none' all weighting functions are turned off. For overlapping inputs each repeating setting overraids the settings made before. The input is case insensitive. Possible selections:
  - trace gas name $\longrightarrow$ O_3 NO_2 SO_2 ClO HCHO BRO NO_3 OCLO O_4 O_2 H_2O CO_2 N_2O CO CH_4 NO NH_3 HNO_3 OH HF HCL HBR HI;
  - 'all' $\longrightarrow$ turns on all trace gas weighting functions;
  - 'none' $\longrightarrow$ turns off all trace gas weighting functions.

  An example of input field is given by the following line:
  ```
  Weighting functions: trace gases
  'R': O3 NO2; 'A': H2O
  ```
  which requires the calculation of relative weighting functions for O_3 and NO_2, and absolute weighting functions for H_2O.
  Attention: Independent of these settings the weighting functions are calculated only for trace gases turned on in the forward model (see "control.inp" file).

- Aerosol weighting function selection.
  The weighting functions for the aerosol can be selected using the input field of the "Weighting functions: aerosol parameters" line. The input field must contain comma or space separated list of aerosol parameters for which the weighting functions need to be calculated. The input is case insensitive. Possible selections:
  - 'aer-ext' $\longrightarrow$ aerosol extinction coefficient;
  - 'aer-sca' $\longrightarrow$ aerosol scattering coefficient;

- 'aer-abs' ⟶ aerosol absorbtion coefficient;
- 'aer-erw' ⟶ aerosol extinction coefficient at a reference wavelength;
- 'aer-dens' ⟶ density of aerosol particles;
- 'aer-modr' ⟶ median radius of particle size distribution function;
- 'aer-var' ⟶ width parameter of particle size distribution function;
- 'aer-modr_f' ⟶ fine mode median radius;
- 'aer-modr_c' ⟶ coarse mode median radius;
- 'aer-var_f' ⟶ fine mode width parameter;
- 'aer-var_c' ⟶ coarse mode width parameter;
- 'aer-cm_frac' ⟶ coarse mode fraction;
- 'all' ⟶ turns on weighting functions for all aerosol parameters listed above;
- 'none' ⟶ turns off weighting functions for all aerosol parameters listed above.

The separation between relative and absolute weighting functions cam be done by the same way as for the trace gas weighting functions (see above).
If the bimodal lognormal particle size distribution function is selected (see Section 3.14.6.1), weighting functions for median radius and width parameter of the fine and coarse mode as well as the weighting function for the coarse mode fraction can be calculated also.
Limitations:

- Only the lognormal particle size distribution function is implemented into current version of the SCIATRAN code.

- Weighting functions for cloud parameters.
If the "Clouds present?" input parameter is set to "t" (see Section 3.15), then the weighting functions for cloud parameters can be selected in the "Weighting functions: cloud parameters" input line as described below. The control parameter "Weighting functions: cloud parameters" input field must contain comma or space separated list of cloud parameters for which the weighting functions need to be calculated. The input is case insensitive. Possible selections are:

```
##  'cld-sca_{x}' => cloud scattering coefficient
##  'cld-abs_{x}' => cloud absorbtion coefficient
##  'cld-lwc_{x}' => cloud liquid water content
##  'cld-pnc_{x}' => cloud particles number density concentration
##  'cld-ref_{x}' => effective radius of water droplets or ice crystal
##  'cld-tau_{x}' => cloud optical thickness
##               (not valid for mixed clouds, see cloud.inp)
##  'cld-cth' => cloud top hight
##  'cld-cbh' => cloud bottom hight
##  'all'     => turns on weighting functions for all cloud
##               parameters allowed in the selected mode
##  'none'    => turns off weighting functions for all cloud
##                     parameters listed above
```

For a water or ice cloud the extension $\{x\}$ should be set to "nomix". In the case of a mixed cloud the extension $\{x\}$ can be set to "water" or "ice". The following example illustrates the input field of this control parameter in the case of non-mixed cloud:

```
Weighting functions: cloud parameters
R: cld-lwc_nomix, cld-ref_nomix, cld-cth, cld-cbh, cld-tau_nomix
```

In this case the program generates weighting functions for vertical profiles of liquid water content and effective radius as well as for cloud top height, bottom height, and cloud optical thickness.

Attention

- If the control parameter "Thermodynamic state" is set to "mixed" the weighting functions will be calculated for water and ice.
- If the parameter "Number of cloud layers" greater than one (multilayered cloud system), the weighting functions will be generated for all cloud layers.
- Weighting functions for CTH, CBH, and optical thickness will be calculated always for absolute variation of corresponding parameters.

The weighting functions for parameter functions will be stored in the directory "./DATA_OUT" under following filenames:

If "Thermodynamic state" is set to "water"/"ice" then	If "Thermodynamic state" is set to "mixed" then
"wf_cld-{ext1}_nomix.dat"	"wf_cld-{ext1}_{ext2}.dat"

where the name {ext1} can be "sca", "abs", "lwc", "pnc" or "ref", and the name {ext2} is "water" or "ice".
Thus, for example, in the case of a mixed cloud the weighting function for effective radius will be stored in two files "wf_cld-ref_water.dat" and "wf_cld-ref_ice.dat". The first file contains weighting function for effective radius of water droplets and the second for the effective radius of ice crystals.

The weighting functions for scalar parameters will be stored in the directory "./DATA_OUT" under following filenames: "wf_cld-{ext1}-{N}.dat", where {ext1} is "CTH", "CBH" or "TAU" (in the case of mixed cloud or multilayer clouds containing water and ice clouds instead of "TAU" will be used "TAU_water" and "TAU_ice" corresponding to the weighting functions with respect optical thickness of water and ice, respectively) and {N} (equal to 1,2,...) defines to which cloud layer belong the corresponding weighting function. We remind that cloud layers are counted from the bottom of the atmosphere to the top.

Limitations: The weighting functions for such cloud parameters as scattering coefficient, absorption coefficient and particle number density can be calculated not for all values of "Type of input integral parameter", i.e.,

```
## ------------------------------------------------------------------------
## |   WF   |'TAU'|'WATER_PATH'|'LWC_PROFILE'|'IWC_PROFILE'|'DENS_PROFILE'|
## | 'sca'  |  -  |     -      |     +       |     +       |      +       |
## | 'abs'  |  -  |     -      |     +       |     +       |      +       |
## | 'lwc'  |  +  |     +      |     +       |     +       |      +       |
## | 'pnc'  |  -  |     -      |     -       |     -       |      +       |
## | 'ref'  |  +  |     +      |     +       |     +       |      +       |
## ------------------------------------------------------------------------
```

```
## Note: not allowed weighting functions are switched off automatically
```

where sign "-" shows that the calculation of the corresponding weighting function is not allowed for this value of the input integral parameter.

- Weighting function for other parameters.
  The weighting functions for other atmospheric parameters can be selected using the input field of the "Weighting functions: other atmopsheric parameters" input line. The input field must contain comma or space separated list of parameters for which the weighting functions need to be calculated. The input is case insensitive. Possible selections:
  - 'Ray' ⟶ Rayleigh scattering;
  - 'Albedo' ⟶ surface albedo;
  - 'ANPS' ⟶ average number of photon scattering events;
  - 'Press' ⟶ pressure profile ;
  - 'Temp' ⟶ temperature profile;
  - 'Elev' ⟶ surface elevation;
  - 'TH' ⟶ tangent height;

  Parameters of PROSAIL BRDF model (reflection by vegetation layer):
  - 'prosail_Ala' ⟶ average leaf angle (for Type=2);
  - 'prosail_Car' ⟶ carotenoid content;
  - 'prosail_Cbr' ⟶ brown pigment content;
  - 'prosail_Cm' ⟶ leaf mass area;
  - 'prosail_Cab' ⟶ chlorophyll content;
  - 'prosail_Cw' ⟶ EWT;
  - 'prosail_LAI' ⟶ leaf area index;
  - 'prosail_PSO' ⟶ soil factor (dimensionless);
  - 'prosail_Stc' ⟶ structure coefficient;

  Parameters of land fluorescence:
  - 'flu_sfl' ⟶ scaling factor for the fluorescence spectrum
  - 'flu_amp-1' ⟶ amplitude first Gaussian Component (GC)
  - 'flu_wlm-1' ⟶ position of maximum first GC
  - 'flu_hwhm-1' ⟶ half width at half maximum first GC
  - 'flu_amp-2' ⟶ amplitude second GC
  - 'flu_wlm-2' ⟶ position of maximum second GC
  - 'flu_hwhm-2 ⟶ half width at half maximum second GC

  General settings:
  - 'all' ⟶ turns on weighting functions for all other parameters listed above;
  - 'none' ⟶ turns off weighting functions for all other parameters listed above.

  The separation between relative and absolute weighting functions cam be done by the same way as for the trace gas weighting functions (see above).

- Weighting function for ocean parameters.
  If the radiative transfer in the atmosphere and ocean is required (key parameter "Include

radiative transfer within ocean or ice" in the control file "control.inp" is set to "ocean"), the weighting functions of following oceanic parameters can be calculated also, setting appropriate flags in control lines "Ocean parameters - weighting functions" to "t"

```
Chlorophyll  Rayleigh  Pm-Us  Pm-Ks  Pm-Kl
    f           t        f      f      f
```

where "Pm-Us", "Pm-Ks", and "Pm-Kl" denote scattering coefficients for small, large, and user defined hydrosol particles, respectively.
Attention: This option is preliminary disabled!

- Representation of weighting functions (absolute/relative).
  Attention: Some weighting functions are not affected by this setting i.e.:
  - the weighting functions for the temperature, surface elevation, tangent height, cloud top height, bottom height, cloud optical thickness as well as the average number of photon scattering events are always **a**bsolute;
  - the pressure weighting function remains always **r**elative.

- Normalization of weighting functions.
  Furthermore, in "DOM_S" mode the normalization of the weighting functions can be changed using the "WF normalization" control parameter. Whereas in the "standard" mode the weighting functions refer to variations of atmospheric parameters within internal altitude layers defined by the input altitude grid, setting the "WF normalization" control parameter to "unified" the weighting functions are renormalized to 1 km altitude layers, i.e., they refer in this case to variations of atmospheric parameters within vertical layers of 1 km extension. The "unified" mode is used for weighting function visualization only and is not appropriate for a retrieval because does not contain the appropriate quadrature coefficients.

Limitations:

- In the current version of SCIATRAN the weighting function for ocean parameters are not properly implemented.
- The calculation of average number of photon scattering events (ANPS) is not possible.
- In the solar/lunar occultation mode (parameter "RTM_TYPE" set to "transmission") only trace gas weighting functions can be calculated (controlled by by the "Weighting functions: trace gases" parameter line). Any settings in
  "Weighting functions: other atmopsheric parameters" or in
  "Weighting functions: aerosol parameters" control lines have no effect.
- If parameter "RTM_CORE" is set to "CDI" weighting functions for pressure, temperature, Rayleigh and aerosol scattering, cloud parameters, surface elevation, as well as average number of photon scattering events (ANPS) are not available. Corresponding settings in "Weighting functions: other atmopsheric parameters" or in
  "Weighting functions: aerosol parameters" control lines have no effect. Albedo weighting function is calculated by means of a numerical perturbation.
- Weighting functions for the tangent height (TH) are only available if parameter "RTM_CORE" is set to "CDI". Otherwise they are switched off independently of the settings in the "control_wf.inp" file.

Attention: Please note, weighting functions are only calculated if corresponding forward model parameter, e.g., absorption by a trace gas, aerosol, clouds, is switched on (see Sec-

tions 3.10, 3.14.1, and 3.15 to learn how to switch forward model parameters on/off).

3.1.7 Rotational Raman scattering in atmosphere ("raman")

Appropriate control files: "control.inp", "control_rrs.inp"
Relevant control parameters:
"Approach to calculate contribution of Raman lines", "Maximum rotational number", "Numerical technique used for RRS", "Raman binning step", "Ring spectra output mode", "Ring spectrum for Stokes component", "Test with single model Fraunhofer line", "Tradeoff speed/memory", "Use spin-rotational splitting"

Setting " RTM Mode" control parameter to "raman", the radiative transfer calculation will be performed accounting for the rotational Raman scattering of atmospheric N_2 and O_2 molecules. The theoretical background and implementation details are given in (**??**).
The calculation of Raman scattering is allowed in line-by-line mode (see Section 3.10.3), ESFT (c-k) mode (see Section 3.10.4), using cross section (see Section 3.10.1), and without gaseous absorption (in Fraunhofer lines). The spectral convolution is possible with any appropriate slit function (see Section 3.11).
Parameters specific for this mode should be selected in the "control_rrs.inp" input file:

- User can switch between two techniques implemented in SCIATRAN to calculate radiative transfer including rotation Raman scattering:
  - setting "Numerical technique used for RRS" control parameter to "dom" the standard discrete-ordinates technique will be used;
  - setting this control parameter to "adj'' the forward-adjoint approach will be employed.
    Attention: Limitations of these techniques are listed below.
- If the " RTM-CORE" control parameter is set to "DOM_V" user can calculate the Ring spectra for all or selected components of Stokes vector setting in the "Ring spectrum for Stokes component" control line "t" or "f":

  ```
  # I  Q  U  V
  Ring spectrum for Stokes component
    t  t  t  f
  ```

  This setting forces the program to calculate Ring spectra for I, Q, and U components of Stokes vector.
- The O_2 RRS cross-section can be calculated accounting for an electron spin-rotational splitting. The splitting will be used if first entry in the "Use spin-rotational splitting" control line is set to "t" (true). Other two entries contain filenames with corresponding spectroscopic information:

  ```
  t, 'DIR/O2_ET-HITRAN-2012.dat', 'DIR/O2_PT-HITRAN-2012.dat'
  ```

  Here "DIR" is the path to the directory where files with spectroscopic information are located.
  Attention: This option requires significantly more computation time.

- The number of Stokes (Anti-Stokes) lines which will be accounted for in calculations should be defined in the "Maximum rotational number" control line.
  Attention:
  - If first entry in the "Use spin-rotational splitting" control line is set to "t", all available transitions of O_2 will be accounted for.
- User can switch between two approachs to calculate the contribution of Raman lines setting in "Approach to calculate contribution of Raman lines" control line "exact matching" or "simple binning". In the first case positions of all Raman lines will be accounted for exactly.
- If control parameter "Approach to calculate contribution of Raman lines" is set to "simple binning" the user needs to define the wide of the spectral bin in "Raman binning step" control line. In this case all Raman lines within this bin have the same spectral position. This option is significantly faster as compare to "exact matching".
- One can select tradeoff between speed of calculation and virtual memory used. Setting in "Tradeoff speed/memory" control line ‘‘speed" or "memory" the user can increase the calculation speed or decrease the needed virtual memory, respectively.
- User can switch between two representations of the calculated Ring spectra setting in the "Ring spectra output mode" "log" or "rel"
  - if "Ring spectra output mode" is set to "log", output will be given as $r(\lambda) = \ln[\, I_+(\lambda)/I_-(\lambda)\,]$
    Attention: this output can be used only in the scalar case;
  - if "Ring spectra output mode" is set to "rel", output will be given as $r(\lambda) = [\, I_+(\lambda) - I_-(\lambda)\,]/I_-(\lambda)$, where $r(\lambda)$ and $I_+(\lambda)$, $I_-(\lambda)$ are ring spectrum, and intensities obtained with and without inelastic scattering, respectively;
  - $r(\lambda)$, $I_+(\lambda)$, and $I_-(\lambda)$ are put into files "./DATA_OUT/ring.dat", "./DATA_OUT/intensity.dat", and "./DATA_OUT/intensity_noring.dat", respectively.

  Attention: This output is possible if "Numerical technique used for RRS" control parameter is set to "adj". If "Numerical technique used for RRS" control parameter is set to "dom", the ring spectra should be calculated by user as discussed below.
- For the test purpose the calculation of Raman scattering can be performed using single model solar line centered at 393.48 nm. This can be done setting in "Test with single model Fraunhofer line" control line "t". The single model Fraunhofer line is defined as follos: $S(\nu) = 1 - 0.82\,(1 - |\nu - \nu_0|/70)$, where $\nu_0 = 25414$ cm^{-1}.

Limitations of the "dom" mode.

- The case of the plane-parallel, "pp_scat", geometry:
  - The "Post-processing type" control parameter should be set to "Interp" (see Sec. 3.7.5), i.e., the solution for all viewing directions which do not match the Gaussian nodes will be obtained by linear angular interpolation instead of the standard post-processing technique.

- The output file "intensity.dat" (see Sec. 3.23.1) contains for this mode the inelastic scattered radiation $I_+(\lambda)$ only, i.e., to obtain Ring spectrum $r(\lambda)$ as defined above, the user need to run SCIATRAN two times, namely, including and excluding Raman scattering to obtain $I_+(\lambda)$ and $I_-(\lambda)$, respectively.
- "Single scattering correction" mode (see Sec. 3.7.5) can not be used in combination with the "dom" technique.

- The case of pseudo-spherical and spherical geometries:
  - In these cases (control parameter "RTM_TYPE" is set to "ps_scat" or "spher_scat") the calculation of rotational Raman scattering is not implemented in SCIATRAN for the "dom" mode. Use the mode "adj" instead.

Limitations of the "adj" mode.

- The case of the plane-parallel, "pp_scat", geometry:
  - The "Post-processing type" control parameter should be set to "Int_SF" (see Sec. 3.7.5), i.e., the solution for all viewing directions which do not match the Gaussian nodes will be obtained by the standard post-processing technique. The angular interpolation technique can not be employed.
  - The parameter "Analytic for conservative scattering", see Sec. 3.7.5, has to be set to "f" (false) in the "control_ac.inp" file. The pseudo-absorber approach can be used only to consider radiative transfer in layers without absorption.
- The case of the pseudo-spherical, "ps_scat", geometry:
  - The rotational Raman scattering is not yet implemented for the case of the pseudo-spherical geometry.

Attention:
To properly calculate rotation Raman scattering check also that:

- the control parameter "Advanced Rayleigh settings" is set to "t" in the file "control.inp";
- the control parameter "Rayleigh scattering index" is set to "4" in the file "control_ray.inp";
- the control parameter "King factor" is set to "from file" in the file "control_ray.inp";
- the file defined in the control line "Rayleigh depolarisation filename" in the file "control_ray.inp" contains data of oxygen and nitrogen anisotropy of polarizability in the required spectral range.

3.1.8 Weighting functions by numerical perturbations ("num_pert")

Appropriate control files: "control.inp", "control_wf.inp"
Relevant control parameters: "RTM Mode", "Lower and upper boundary for WF calculation", "Numerical perturbation of water/ice", "Numerical perturbation with respect to"

Setting "RTM Mode" control parameter to "num_pert" allows some weighting functions to be calculated using the numerical perturbation technique. The altitude range to calculate the numerical weighting functions is defined by the "Lower and upper boundary for WF calculation" control parameter in the "control_wf.inp" input file.
Attention: **This mode is intended for developing and test purposes only and should not be invoked by ordinary users.**

3.1.9 Retrieval ("ret")

Appropriate control files: "control.inp", "control_ret.inp"

Setting "RTM Mode" control parameter to "ret", the retrieval of various atmospheric parameters (i.e., vertical distributions of atmospheric trace gases) can be performed. Retrieval parameters are to be specified in "control_ret.inp" file. A detailed description of the retrieval modes and corresponding parameters can be found in Chapter 4.

3.2 Extra-terrestrial solar flux (irradiance)

Appropriate control file: "control.inp"
Relevant control parameters: "Extra-terrestrial solar flux", "Filename user provided solar spectrum", "Dimension of extra-terrestrial solar flux".

In order to start radiative transfer calculation one needs to define the incoming solar flux at the top of atmosphere. The extra-terrestrial solar flux should be defined setting in "Extra-terrestrial solar flux" input line "File", "Pi" or "Unity".

- If "Extra-terrestrial solar flux" parameter is set to "File",
  the solar spectrum will be read from an external file. The filename (including path to the directory containing corresponding files) of irradiance spectrum should be given in the "Filename user provided solar spectrum" control line. This file consists of a header and two columns. All lines beginning with "#" will be considered by program as header lines. First column contains wavelength and second column contains solar spectrum.
  Dimension of the wavelength and irradiance should be given in the
  "Dimension of extra-terrestrial solar flux" control line. The example of this control line and input field is given below. The input field consists of the six entries:

```
##      Entry     Variable      Allowed dimension
##      ------------------------------------------------------------
##       1       Wavelength       [nm],[micron]
##       2     'air' or 'vac'     input wavelength in air or vacuum
##       3        Power           [W],[phot/s]
##       4        Area            [m^2],[cm^2]
##       5     Spec. Interval     [nm],[micron]
##       6     Scaling factor        optional (can be not presented)
##      ------------------------------------------------------------
##  WL    air/vac    Power      Area       Spec.   Scaling
##   1       2         3         4       interval   factor
Dimension of extra-terrestrial solar flux
   'nm'    'air'      'W'      'cm^2'      'nm'     1.d-6
```

  The dimension of the solar flux is [Power]/[Area]/[dλ], where allowed dimensions of [Power], [Area], and [dλ] are given in the table above. The scaling factor can be used if e.g., the input file contains [Power] of the solar flux in [mW] or [μW].
  Attention:
  - The wavelength in the file containing solar spectrum can be given in air or vacuum.

- The scaling factor 1.d-6 in the example of the input field was used to recalculate [μW] in [W].
- The program requires information about dimension of the input solar spectrum to properly calculate the Planck function and trans-spectral energy transport in the case of thermal emission or any inelastic scattering process, e.g., rotational Raman scattering.

User can find different irradiance spectra in the SCIATRAN database, e.g.,
"SES_E490.dat" - 2000 ASTM Standard Extraterrestrial Spectrum Reference E-490-00 (see http://rredc.nrel.gov/solar/spectra/am0/ASTM2000.html) in the spectral range 0.12 - 400 μm expressed in [W/m^2/μm] or
"thkur.dat.gpp" - irradiance spectrum created from MODTRAN data in the spectral range 200 - 2500 nm expressed in [phot/s/cm^2/nm].

- If "Extra-terrestrial solar flux" parameter is set to "Pi" or to "Unity" and no thermal emission or inelastic scattering processes is required the solar irradiance is supposed to be equal π or 1, respectively, at all wavelengths. The output units are any appropriate intensity units, e.g., W m^{-2} nm^{-1} sr^{-1}.
  Attention:
  - The control line "Dimension of extra-terrestrial solar flux" will be ignored by the program if "Extra-terrestrial solar flux" parameter is set to "Pi" or to "Unity".
  - If thermal emission should be taken into account the "Extra-terrestrial solar flux" parameter will be set automatically to "File".

3.3 Main altitude grid

Appropriate control file "control.inp"
Relevant control parameters: "Altitude grid file name", "Height above sea level"

To perform radiative transfer calculations through vertically inhomogeneous medium an user must define the main altitude grid which will be used by the program in all calculations.
In the "Altitude grid file name" input line the file name containing the altitude grid for radiative transfer calculation is to be specified. The input line contains the path and the name of the file containing the altitude grid. Altitudes in the grid file (in [km]) should be arranged as a column and must be monotonously increasing or decreasing.
The main altitude grid can be also defined directly in the input field after control parameter "Altitude grid file name" as follows:

```
0.   2.  10.  30.  60.
  0.5   2.   5.   10.
```

First input line contains values of discrete altitude levels ($\geq$ 2) in [km], and second line conteins steps (in [km]) which will be used by the program to introduce additional altitude levels between givne in first line. Thus, the resulting main altitude grid corresponding to the input above is
[0. 0.5 1. 1.5 2. 4. 6. 8. 10. 15. 20. 25. 30. 40. 50. 60.]

The top of atmosphere (TOA) in the radiative transfer model is set to the maximum height level in the altitude grid.

Setting "Height above sea level" parameter to a value large than 0 km one can cut off the atmosphere below the selected height simulating measurements, for example, over mountains. The altitude grid above this selected height will be not changed.
Attention:

- The number of altitude layers defines the speed of calculations. Therefore, the choice of altitude grid depends in the first line on the vertical inhomogeneity of the atmosphere.
- The main altitude grid and the number of altitude layers will be changed by the program if the parameter "Clouds present?" in the "control.inp" file is set to "t" (see Section 3.15) or the "Aerosol as a cloud layer?" control parameter in the "man_aer.inp" file is set to "yes" (see Section 3.14.5).

3.4 Sphericity of the atmosphere

Appropriate control files: "control.inp", "control_geom.inp", "control_ac.inp"
Relevant control parameters: "RTM_TYPE"

Setting "RTM_TYPE" to "spher_scat", "pp_scat", or "ps_scat", the solar radiation scattered by the Earth's atmosphere and reflected from the surface is simulated. Depending on the selected parameter the shape of the atmosphere is considered to be either spherical or plane-parallel and can be different for the direct solar beam and the scattered light. Possible selections are discussed in details in the following subsections.
Setting "RTM_TYPE" control parameter to "vhl", a specific case of radiative transfer in a vertically homogeneous layer can be used. In this case in the framework of plane-parallel approximation many input parameters of SCIATRAN will be installed automatically by the program (see Section 3.4.2).

3.4.1 Plane-parallel atmosphere ("pp_scat")

Appropriate control file: "control.inp"
Relevant control parameters: "RTM_TYPE", "RTM-CORE"

The plane-parallel mode is active if "RTM_TYPE" parameter is set to "pp_scat". All radiative transfer calculations are performed in a plane-parallel atmosphere, i.e., all effects due to the sphericity of the Earth's atmosphere are neglected. This mode is recommended to simulate daylight measurements in near zenith or near nadir viewing geometry.

Limitations:

- The mode is not supported if "RTM-CORE" is set to "CDI" (automatically switched to pseudo-spherical mode).
- Increasing errors for solar zenith angles larger than $\sim 75°$.
- Approximation is not valid for solar zenith angles larger than/equal to $90°$.
- Increasing errors for line-of-sight angles larger than $\sim 20°$ depending on solar zenith angle, wavelength, etc..
- This mode is not appropriate for limb viewing geometry.

3.4.2 Vertically homogeneous layer ("vhl")

Appropriate control files: "control.inp", "control_geom.inp", "control_ac.inp", "control_out.inp", and "man_vhl.inp"
Relevant control parameter: "RTM_TYPE"

The plane-parallel mode is also active if "RTM_TYPE" parameter is set to "vhl". All radiative transfer calculations are performed in a plane-parallel vertically homogeneous layer. This mode is recommended especially for unexperienced users because many input control parameters of SCIATRAN will be set automatically by the program. In particular, user needs to perform following settings only:

- set optical properties of a homogeneous layer, i.e., optical thickness, single scattering albedo, and scattering function/matrix using separate input file "man_vhl.inp";
- set parameter "RTM-CORE" to "DOM_S" or "DOM_V" (in the file "control.inp") to select RT calculations in the scalar or vector mode, i.e., excluding or including polarization;
- set parameter "Extra-terrestrial solar flux" to the desired value in the file "control.inp";
- select reflection type at the lower boundary of the layer setting "Surface reflection type" to the desired reflection type in the file "control.inp";
- set illumination and observation geometry, i.e., solar zenith angle, viewing zenith angle, relative azimuthal angle, and observer position in the input file "control_geom.inp" (see Section 3.8).

The additional setting should be done to control speed and accuracy of RT calculations as well the layout and format of output data. For these purpose the user can select the default mode or

- set output layout and format using the control file "control_out.inp" (see Section 3.22.1);
- set accuracy and speed of radiative transfer calculations in the file "control_ac.inp" (see Section 3.7).

The default mode is active if control parameters "Advanced accuracy control" and "Output format specification" are set to "f" in the file "control.inp".

3.4.2.1 Input file "man_vhl.inp"

If the "vhl" mode in the "control.inp" file is selected, then the optical parameters of a homogeneous layer have to be defined by user in the file "man_vhl.inp". There are following options:

- Select input form of scattering function/matrix.
  Using the "Scattering function representation" input line user can switch between three possibilities to import scattering function/matrix into SCIATRAN:
  - "Asymmetry_factor" - the scattering function is defined by the asymmetry factor according to the Henyey-Greenstein parameterization. The desired value of the asymmetry factor should be given in "Asymmetry factor value" input line.
  - "Expansion_coeff" - the scattering function is represented by the Legendre or spherical functions series expansion coefficients in the scalar or vector case, respectively.

The filenames containing the expansion coefficients should be specified in the "File name containing expansion coefficient" input line. The path to the directory containing corresponding files should be given in "Directory name for scattering matrices" input line. The file containing expansion coefficients is formatted as follows:

```
Example of the file containing expansion coefficients
Numerical accuracy = 0.10D-06
CEXT   = 0.339753D+01; CSCA  = 0.339753D+01
ALBEDO = 0.10D+01;     <COS> = 0.783276D+00
   S     ALPHA 1   ALPHA 2   ALPHA 3   ALPHA 4   BETA 1   BETA 2
>
   0     1.000      0.000     0.000     0.915     0.000    0.000
   1     2.104      0.000     0.000     2.095     0.000    0.000
   2     2.095      3.726     3.615     2.008    -0.116    0.065
   3     1.414      2.202     2.240     1.436    -0.209    0.221
   4     0.703      1.190     1.139     0.706    -0.227    0.097
   5     0.235      0.391     0.365     0.238    -0.144    0.052
   6     0.064      0.105     0.082     0.056    -0.052    0.009
```

In this example first 6 lines will be considered as comment lines. In fact the number of comment lines in the file header is arbitrary. Each line containing any character except of $0, 1, \ldots, 9$, E, e, D, d will be considered as a comment line. The first column in the data block (after line beginning with >) has to be presented but is not used. The number of lines in the data block corresponds to the number of moments needed for the appropriate representation of scattering function/matrix (only seven lines is shown in the example above). The subsequent data block contains the expansion coefficients in the second column and in 2-7 columns in the scalar and vector case, respectively.

Attention:

- The reading of moments (lines) in this file will be finished if
  - end-of-file is reached;
  - expansion coefficient in a line is zero;
  - the number of read moments greater than 5000.

- "Scattering_matrix" - the scattering function is given as a function of the scattering angle. The filename containing scattering function should be specified in the "File name containing scattering function/matrix" input line. The path to the directory containing corresponding files should be given in "Directory name for scattering matrices" input line. The parameterization has to be supplied in a file which is formatted as follows. The subsequent data block contain scattering angles in degrees in the first column and appropriate values of the phase function in the second column.

  Limitation:

  - this option is not supported in the vector case.

- Optical thickness of the layer.
  The optical thickness of the layer should be set in the "Optical thickness" control parameter.

- Single scattering albedo of the layer.
  The single scattering albedo of the layer should be set in the "Single scattering albedo (VHL)" control parameter.

Attention:

- Some options of RT calculations as, for example, spectral dependent surface albedo or BRDF require wavelength to define corresponding wavelength dependent parameters. It is assumed that in the case of "vhl" mode all needed wavelength dependent parameters will be used by the program for the wavelength 500 nm.

3.4.3 Pseudo-spherical atmosphere ("ps_scat")

Appropriate control file: "control.inp"
Relevant control parameters: "RTM_TYPE", "RTM-CORE"

The pseudo-spherical mode is active if "RTM_TYPE" parameter is set to "ps_scat". In this mode the radiative transfer equation is solved in the plane-parallel atmosphere whereas the single scattering source term is calculated in spherical geometry, i.e., the ray tracing for the direct solar beam is performed assuming a spherical atmosphere. This mode is recommended e.g., to simulate measurements of the scattered solar radiation during the twilight in near zenith or near nadir viewing geometry.
Limitations:

- Increasing errors for solar zenith angles larger then $\sim 92°$.
- Increasing errors for line-of-sight angles larger then $\sim 30°$ depending on solar zenith angle, wavelength, etc..
- This mode is not appropriate for limb viewing geometry.

Attention:

- The pseudo-spherical mode, "ps_scat", is automatically switched on if "RTM-CORE" is set to "CDI" in the plane-parallel mode ("RTM_TYPE" set to "pp_scat").

3.4.4 Spherical atmosphere ("spher_scat")

Appropriate control file: "control.inp"
Relevant control parameters: "RTM_TYPE", "RTM-CORE", "The number of iterations"

The spherical mode is active if "RTM_TYPE" control parameter is set to "spher_scat". In this mode, an accurate spherical ray tracing approach is employed to compute the single scattered radiation whereas an approximation is used to obtain the multiple scattering contribution. The method to account for the multiple scattering as well as to calculate the weighting functions depends on the setting of the "RTM-CORE" control parameter. For further details see Sec. 3.6.

If "RTM-CORE" control parameter is set to "CDI", the accuracy of the multiple scattering approximation is controlled by "The number of iterations" control parameter whereas in the "DOM_S" or "DOM_V" mode this parameter is always set to its default value of "1".
Setting "The number of iterations" control parameter to "1" results in approximated spherical

solution based on the estimation of the multiple scattering contribution using the solution of the radiative transfer equation in the pseudo-spherical atmosphere at appropriate solar zenith angles (as done, for example, in the CDI radiative transfer model). This is a quick spherical approximation which is sufficient for most of geophysical applications.
Setting "The number of iterations" to a value large than "1" leads to successive iterations of the multiple scattering radiation field in the spherical atmosphere (CDIPI radiative transfer model). This is a quite time-consuming procedure, the computing time is linearly increasing with the "The number of iterations" value. Setting ''The number of iterations" to "2" is in most cases sufficient to obtain a fully spherical solution with a suitable accuracy. However, this setting has only an effect for the radiance, whereas the approximation for the weighting functions remains unaffected.
Limitation:

- The multiple scattering is set to zero for solar zenith angles large than 98°.

3.4.4.1 Solar/lunar occultation mode

Setting "RTM_TYPE" to "transmission" the solar/lunar occultation mode is selected, i.e., the direct solar radiation transmitted through the Earth's atmosphere is simulated. In this mode, the Earth's atmosphere is always considered to be spherical.

3.4.4.2 Refraction

Appropriate control file: "control_geom.inp"
Relevant control parameters: "Refractive geometry", "Earth radius"

The curvature of the Earth's atmosphere is defined by the "Earth radius" parameter in "control_geom.inp" which should be specified in [km]. The refraction effect can be considered in the ray tracing calculations for the direct solar beam in the pseudo-spherical mode, and in all ray tracing calculations (including scattered light) in the spherical mode setting first entry in the "Refractive geometry" control line to "t" in the "control_geom.inp" input file.
If the first parameter is set to "t" atmospheric refraction will be taken into accout (not in plane-parallel geometry). The second parameter defines the wavelength in [nm] to calculate the refractive index.
Optionally, maximum altitude in [km] and minimum solar zenith angle in [deg] can be specified as the third and the fourth entries, respectively. The refraction for the direct solar light is accounted for only at altitides below the maximum value and solar zenith angles larger than the minimum value. If no input is provided default values of 35 km and 70° are used.
Limitations:

- No wavelength dependence of the air refraction index is implemented.

3.5 Radiative transfer through ocean or ice

Appropriate control file: "control.inp"
Relevant control parameters: "Include radiative transfer within ocean or ice"

The radiative transfer processes can be considered employing the SCIATRAN model not only in the terrestrial atmosphere bounded by a reflecting surface but also within ocean or ice including coupling between atmosphere and corresponding medium.

- Atmosphere underlying surface.
  Setting "Include radiative transfer within ocean or ice" control parameter to "none", the radiative transfer will be considered in the atmosphere bounded by reflecting or perfectly absorbing surface. The surface reflection properties included in SCIATRAN are given in Secs. 3.16 - 3.16.2.3.
- Coupled ocean-atmosphere model.
  Setting "Include radiative transfer within ocean or ice" control parameter to "ocean", the radiative transfer will be considered in the ocean-atmosphere system. Detailed considerations are given in Sect. 3.20.
- Coupled ice-atmosphere model.
  Setting "Include radiative transfer within ocean or ice" control parameter to "ice", the radiative transfer will be considered in the ice-atmosphere system. Detailed considerations under preparation.

3.6 Radiative transfer solvers

Appropriate control file: "control.inp"
Relevant control parameters: "RTM-CORE"

Using the "RTM-CORE" control parameter users can switch between different methods to solve the radiative transfer equation and to calculate the weighting functions. The option has no effect if "RTM_TYPE" parameter is set to "transmission" (see Section 3.4.4.1).

3.6.1 Fully featured solvers ("CDI" and "DOM_S", "DOM_V")

Appropriate control file: "control.inp"
Relevant control parameters: "RTM-CORE"

The user can swith between three solvers of radiative transfer equation, i.e., "CDI", "DOM_S" and "DOM_V". The choice depends on the particulate problem to be solved.

- Solver "CDI".
  Setting the "RTM-CORE" control parameter to "CDI", the CDI/CDIPI radiative transfer model (Rozanov et al., 2000, 2001) is selected. The "CDI" solver can only be used in the pseudo-spherical and spherical modes, i.e., the "RTM_TYPE" control parameter can only be set to "ps_scat" or "spher_scat", otherwise the pseudo-spherical mode is selected automatically. In the framework of this method, first the entire radiation field as well as, if necessary, the field of weighting functions is calculated in the pseudo-spherical approximation for a set of solar zenith angles using the finite difference method. Thereafter, an integration along the line-of-sight is performed accurately calculating the single scattering contribution and using the pseudo-spherical radiation field to account for the multiple scattering contribution. Depending on the "RTM_TYPE" control parameter setting, the integration along the line-of-sight is performed either for a plane-parallel ("RTM_TYPE"

is set to "ps_scat") or for a spherical ("RTM_TYPE" is set to "spher_scat") atmosphere, whereas during the integration along the direct solar beam the sphericity of the Earth's atmosphere is always accounted for. The weighting functions are calculated using the same method as for the radiance. As described in Sec. 3.4.4, the treatment of the sphericity in the multiple scattering contribution can be improved setting "The number of iterations" control parameter to higher values. However, this makes an effect only for the radiance, whereas the approximation for the weighting functions remains unaffected.
Limitations:

- scalar version is available only (no polarization);
- no coupled ocean-atmosphere mode;
- plane-parallel mode in not supported;
- computationally inefficient in the pseudo-spherical mode;
- clouds are not supported;
- only Henyey-Greenstein phase function is supported for aerosols;
- no delta-M/delta-fit approximation is possible;
- adaptive grid approach can not be used see Section 3.7.3;
- weighting functions are available for trace gas concentrations only.

- Solvers "DOM_S" and "DOM_V".
Setting the "RTM-CORE" control parameter to "DOM_S" or "DOM_V", the discrete ordinates technique is selected. "'DOM_S" and "'DOM_V" are used for scalar and vector (polarized) radiative transfer computation. These solvers can be used in any sphericity mode (any setting of "RTM_TYPE"). The weighting functions are obtained using the solution of the adjoint radiative transfer equation. In the spherical mode, the intensity/Stokes vector is calculated similar to the "CDI" mode, i.e., performing the integration of the multiple scattering source function along the line-of-sight.
Limitations:
  - the case of incident polarized light (e.g., laser) is not supported;
  - the extinction matrix is considered as scalar (only the case of randomly oriented particles is considered);
  - the 3-D effects are not treated;
  - an iterative scheme to improve the sphericity treatment in the multiple scattering term is not available;
  - photochemically active species can not be accounted for, see Sec. 3.12.2.5;

3.6.2 Asymptotic intensity at TOA ("ASYMP")

Appropriate control files: "control.inp", "cloud.inp"
Relevant control parameters: "RTM TYPE", "Clouds present"

Setting the "RTM-CORE" control parameter to "ASYMP" an effective approximation for the radiative transfer modeling in a presence of clouds based on an asymptotic radiatiev transfer theory (Kokhanovsky and Rozanov, 2004) is used in calculations. This mode is extremely fast as compare to the standard radiative transfer calculations but has a number of limitations:

- it can not be used in a cloud-free atmosphere, i.e., "Clouds present" parameter must be set to "t" in the "control.inp" input file;

- the accuracy of this approximation depends on cloud optical thickness and gaseous absorption;
- the calculation of the reflection function at the top of atmosphere is possible (no transmission calculations);
- the polarization effects are not included;
- it can be used in the plane-parallel atmosphere only ("RTM_TYPE" is set to "pp_scat"), see Section 3.4;
- only one cloud layer is supported, i.e., "Number of cloud layers" must be set to "1" (see Section 3.15.1);
- only user-defined type of phase function can be selected, i.e., parameter "Phase function of cloud layers" must be set to "user" (see Sections 3.15.2-3.15.4).

The accuracy of this approximation should be checked by user for required computation scenarios.

3.7 Accuracy of radiative transfer calculation

Appropriate control file: "control_ac.inp".

All parameters related to the accuracy of calculation can be install using default setup if in the file "control.inp" in the "Advanced accuracy control" input line one set "f" (.false.). The default values of all parameters are given below in bracets using the following color. Otherwise ("t" in "Advanced accuracy control" input line) the parameters related to the accuracy should be specified by user in the file "control_ac.inp".

3.7.1 Scattering modes

Relevant control parameters: "Scattering mode" ("ms"), "SS/MS wavelength boundary"

The parameter "Scattering mode" allows user to reduce the computation time switching off the multiple scattering contribution to radiance and/or weighting functions. The following modes are implemented:

- "ms" - fully multiple scattering treatment (default mode);
- "dir_ref" - reflected direct solar light, both intensity/radiance and weighting functions are calculated ignoring all scattering processes. This option has a number of limitations:
  - This mode is supported if "RTM-CORE" parameter is set to "DOM" only.
  - Weighting functions can be calculated for concentration of gaseous absorbers, temperature profile, Lambertian surface albedo, and scaling parameter of the land fluorescence spectra (see Section 3.17) only.
  - Top of atmosphere observation geometry (see "Position of the instrument" in Section 3.8.2) is supported only.
  - Attenuation of the direct solar light caused by aerosol, cloud, and Rayleigh will be accounted for if corresponding component is switched on.
  - This mode is implemented for the plane-parallel geometry only (see Section 3.4.1).
  - This mode can not be used if thermal emission is switched on (see Section 3.19) or coupled ocean-atmosphere model is used (see Section 3.20).

- "ss" - single scattering mode, both intensity/Stokes vector and weighting functions are calculated considering single scattering contribution only;
- "wf_ss" - weighting functions are calculated considering the single scattering contribution only, whereas intensity/radiance is obtained from the fully multiple scattering treatment as in "ms" mode;
- "ss_ms" - calculations are performed in "ss" mode at wavelengths shorter than the wavelength specified in "SS/MS wavelength boundary" input field (see below), "ms" mode otherwise;
- "wf_ss_ms" - calculations are performed in "wf_ss" mode at wavelengths shorter than the wavelength specified in "SS/MS wavelength boundary" input field (see below), "ms" mode otherwise.
- "sm_wf_ss" - calculations are performed in the "ss_ms" mode for the intensity, whereas the weighting functions are calculated considering the single scattering contribution only.

Limitations:

- If the "RTM-CORE" parameter is set to "DOM_S " or "DOM_V", see Section 3.6:
  i) The discrete ordinate solver in the case of plane-parallel, "pp_scat", or pseudo-spherical, "ps_scat", mode supports only the fully multiple scattering, single scattering, and reflected direct solar light mode. ("Scattering mode" parameter can only be set to "ms", "ss", "ss_ms", and "dir_ref"). The surface reflection of the direct solar light is accounted for.
  ii) The discrete ordinate solver in the case of spherical geometry, "spher_scat", supports all modes except "dir_ref". The surface reflection of the direct solar light is accounted for.
- If the "RTM-CORE" parameter is set to "CDI":
  If the multiple scattering contribution is turned off and "RTM-CORE" parameter is set to "CDI" (see Section 3.6) then no surface reflection is considered.

A boundary wavelength in [nm] (set in "SS/MS wavelength boundary" input field) is used to switch automatically between single scattering and multiple scattering modes ("ms_ss", "'wf_ms_ss", and '"sm_wf_ss").

3.7.2 Sub-layers

Relevant control parameters:
"The number of fine grid layers" ("5"), "Fine grid start" ("1"), "Fine grid tangent" ("5"), "Fine grid height" ("3.0"), "Solar fine grid height" ("3.0"), "The layering of line-of-sight" ("2 1 1.0")

The accuracy of the radiative transfer calculations in a presence of a strong vertical inhomogeneity can be increased dividing the altitude layers as given by the main altitude grid into sub-layers. The number of sub-layers per original altitude layer is defined by "The number of fine grid layers" parameter. The following four parameters define altitude regions where the sub-layering is to be done:

- "Fine grid start" - the number of altitude layers corresponding to the original grid which will be divided into sub-layers starting from the first point of the integration line. The

integration line represents commonly the instrument line-of-sight or the lightpath of the direct solar beam.

- "Fine grid tangent" - the number of altitude layers corresponding to the original grid above the tangent height of the integration line (or above the surface) which will be divided into sub-layers.
- "Fine grid height" - all altitude layers corresponding to the original grid below the selected altitude will be divided into sub-layers.
- "Solar fine grid height" - all altitude layers corresponding to the original grid below the selected altitude will be divided into sub-layers along the direct solar beam.

Attention:

- These settings have no effect in a plane-parallel atmosphere ("RTM_TYPE" is set to "pp_scat", see Section 3.4).

Limitation:

- If the discrete ordinate solver ("RTM-CORE" is set to "DOM_S" or "DOM_V", see Section 3.6) is used in the pseudo-spherical mode ("RTM_TYPE" is set to "ps_scat"), the sub-layering is only performed for the direct solar beam.

If the weighting functions in a spherical mode ("RTM_TYPE" is set to "spher_scat") need to be calculated using the discrete ordinate solver ("RTM-CORE" is set to "DOM_S"), an additional griding along the line-of-sight is required, which determines the parts of the line-of-sight where the solar zenith angle is assumed to be constant.
This griding is defined using the "The layering of line-of-sight" control line. The first and the second values in this input line define the number of discrete layers along the line-of-sight before and after the tangent point whereas the third value specifies the vertical extension of these layers. For, example, if an input line "3, 2, 0.5" is specified for a line-of-sight with a tangent height of 10 km, the line-of-sight will be divided into the following pieces: from TOA to 11 km altitude, form 11 km to 10.5 km altitude, from 10.5 km to 10 km altitude, from 10 km to 10.5 km altitude (back side), and from 10.5 km altitude to TOA (back side). Note that both outermost layers extend until the top of the atmosphere independent of the vertical extention specified in the "The layering of line-of-sight" control line. In each of these pieces the weighting functions will be calculated for a constant value of the solar zenith angle.

Attention:

- This setting has only an effect in program modes which include quasi-analytical calculations of weighting functions, i.e., "RTM Mode" is set to "wf", "block_amf", or "ret", see Section 3.1.

3.7.3 Adaptive grid within Discrete Ordinates Method

Relevant control parameters: "Adaptive grid", "Homogeneity criteria"

If the discrete ordinates method is employed ("RTM-CORE" is set to "DOM_S" or "DOM_V", see Section 3.6) the radiative transfer calculations can be substantially accelerated without noticeable lost of the accuracy setting the "Adaptive grid" parameter to "t".
In this mode, the vertical inhomogeneity of the atmosphere is analyzed by the program and altitude layers with not too much different values of the single scattering albedo are joined

into one layer reducing, thus, the dimension of the radiative transfer problem to be solved.
The criterion to decide whether the single scattering albedos of two adjacent layers are too much different is selected setting the "Homogeneity criteria" to an appropriate value which defines the maximum relative difference between the single scattering albedos of the layers to be joined.
Thus, for example, if the "Homogeneity criteria" control parameter is set to "0.2", two layers will be joined if the relative difference between their single scattering albedos is less than 20%.

Limitation:

- not implemented yet in the coupled ocean-atmosphere model.

3.7.4 Fourier series expansion

Relevant control parameters: "Azimuth series flag"("t"), "Do only 0th harmonic for near nadir"("t"), "Near nadir definition [deg]"("0.01"), "Accuracy criterion"("0.001"), "Number of streams"("16"), "Number of Legendre moments"("35")

Attention: All settings discussed in this section have only an effect if the Discrete Ordinate solver is used, i.e., the "RTM-CORE" control parameter is set to "DOM_S" or "DOM_V" (see Section 3.6).

There are following options:

- Number of scattering function/matrix Fourier series term to be used.
  The number of Legendre moments retained in the Legendre series expansion of the scattering phase function is controlled by the "Number of Legendre moments" input parameter.
- Zenith angle discretization.
  The input parameter "Number of streams" controls the number of Gaussian nodes used to discretize the angular integrals in the radiative transfer equation.
  Attention:
  - The selected value should be greater than at least 0.43×("Number of Legendre moments" - 1).
- Convergence control of Fourier series.
  If "Azimuth series flag" parameter is set to "t" the number of Fourier terms considered in radiative transfer calculations will be automatically determined based on the desired accuracy specified in the "Accuracy criterion" control line. The calculation will be finished if the relative contribution of two following harmonics is smaller than the value of criterion in "Accuracy criterion" input line.
  Thus, for example, if the "Accuracy criterion" control parameter is set to "0.01", the calculation will be finishd if the relative contribution of two subsiquent harmonics is less than 1%.
  If "Azimuth series flag" parameter is set to "f" only zeroth harmonic will be taken into account.
- Near nadir approximation.
  Setting the "Do only 0th harmonic for near nadir" control parameter to "t" results in calculating only the zeroth Fourier term in near-nadir geometry, i.e., if all specified viewing angles or all specified solar zenith angles (see Section 3.8.1) are less than the

value specified in "Near nadir definition [deg]" input line. This is true in the scalar case and in both satellite and ground based observation modes.

3.7.5 Additional options

Relevant control parameters: "Accuracy of STA " ("0.1d0"), "Analytic for conservative scattering" ("f 1.d-4") "Check STA" ("f"), "Integration nodes" ("f"), "Integration over L-of-S in Fourier space?" "yes" "Post-processing type" ("Int_SF"), "Precision mode for eigenvalue problem" ("doubl"), "Pre-calculate line-of-sight geometry" ("f"), "Solar grid" ("DB"), "Single scattering correction" ("f"), "Use constant angles along line-of-sight" ("f")

- Post-processing type.
  The "Post-processing type" control parameter is used to define the post-processing type of the discrete-ordinates calculation.
  Setting this parameter to "Int_SF", one forces the program to perform standard post-processing, i.e., integration of the source function along line-of-sight directions. This enables the exact solution for all viewing direction which do not match the Gaussian nodes to be obtained.
  Setting the "Post-processing type" control parameter to "Interp", the standard post-processing will be replaced by the interpolation of radiation field, i.e., the solution for all viewing directions which do not match the Gaussian nodes will be obtained by linear angular interpolation.
  Attention:
  - The standard post-processing technique can not be used if vibrational Raman scattering (VRS) and/or fluorescence are included (preliminary restriction). Therefore, the mode "Interp" is implemented to calculate radiation field with the same approximation exciding inelastic processes if the relative contribution of the corresponding inelastic process should be estimated.

  - The "Post-processing type" control parameter is irrelevant if the "RTM_TYPE" control parameter is set to "spher_scat" (see Sec. 3.4). In this case the program performs numerical integration of the source function along line of sight.

- Single scattering correction technique.
  Single scattering correction technique allows to reduce error introduced by the truncation of scattering function/matrix in Fourier series expansion. The single scattering correction activated by setting the "Single scattering correction" control parameter to "t". The correction is performed by subtracting from the total scattered intensity the single scattering contribution calculated employing an "approximate" phase function (i.e., limited number of Legendre moments are retained in the Legendre series expansion of the phase function) and then adding the single scattering contribution calculated employing the "exact" phase function.
  Limitations:
  - not recommended in combination with SCIATRAN aerosol database (see Section 3.14.3);
  - not implemented yet in the coupled ocean-atmosphere radiative transfer model.
  - can not be used in combination with rotational Raman scattering if "Numerical technique used for RRS" control parameter is set to "dom".

- Treatment of conservative scattering.
  The user can switch between two options to calculate radiative transfer in the layers without absorption (so called conservative scattering, when single scattering albedo equals to 1). Setting in the first entry field of the "Analytic for conservative scattering" input line "t" or "f", the analytical solution or pseudo-absorber approach, respectively, will be employed.
  If "Analytic for conservative scattering" is set to "t", then an analytical solution will be used following the Chandrasekhar technique in layers where absorption probability β = (1 - single scattering albedo) is less than a minimal value β^*. The second entry will be used by the program as β^*;
  If "Analytic for conservative scattering" is set to "f", then the second entry will be interpreted by the program as an absorption probability of a pseudo-absorber.
  Attention:
  - to calculate the weighting function in the case of conservative scattering the "Analytic for conservative scattering" control parameter should be set to "f", i.e., pseudo-absorber approach has to be used:
    ```
    f  1.d-4
    ```
  - It is recommended to set the "Analytic for conservative scattering" control parameter as
    ```
    t  1.d-7
    ```
    to calculate the air mass factors with enhanced accuracy.
- Precision mode for eigenvalue problem.
  Select precision mode which will be used by the program to solve the main DOM eigenvalue problem. The "Precision mode for eigenvalue problem" control parameter can be set to "doubl" or "sngl".
  - the option "sngl" converts the double precision real matrix to a default real.
  - the option "doubl" uses the double precision real matrix. This option is recommended by calculation of the air mass factors of very weak gaseous absorber (see Sect. 3.1.4).

- Accuracy of spherical transmission approximation.
  The accuracy of Spherical Transmission Approximation (STA) can be selected setting in the "Accuracy of STA" control line a desired value of required accuracy in [%].
  To check STA the user needs to set "t" in "Check STA" control line. In this case the program calculates the spherical transmission only and stops. Output file is written out in "./DATA_OUT/appr_spher.out".

- Use constant angles along line-of-sight.
  If "t" is set into the "Use constant angles along line-of-sight" control parameter, then solar, zenith, and azimuthal angles will be set to constant along line-of-sight. These constant values correspond to values at the beginning of line-of-sight. This option enables the impact of solar, zenith, and azimuthal angles variability to be estimated.

- Select solar grid.
  The control parameter "Solar grid" enables default or user defined solar grid which will be used for interpolation of radiation field on the local solar angles along line-of-sight to

be selected:
"Full_DB" - "standard" grid (as given in MODULE GRIDS) is used. Second entry will be ignored.
"Opt_DB" - "standard" grid as defined in modules.f is truncated at the higherst required SZA above 90 deg (no truncation for lower SZAs).
"One" - only one solar zenith angle is used for calculations (average of SZAs at TH or BOA for downward pointing LOS and for the first poit for upward pointing LOS over all line-of-sights defined in the "control_geom.inp").
"UD" - user-defined grid is used. Second entry defines number of discrete angles (minimum 3) between minimal and maximal solar angles for all line-of-sights (equidistand over the cosine of SZA).

- Integration nodes.
  Integration nodes for the angular integration over the unit sphere. Per default the integration is performed using 100 integration nodes which are stored in the program source code. Setting the first entry "Integration nodes" control parameter to "t" the integration nodes are read from the input file. The name of the file must be specified in the second entry of the input field.

- Pre-calculate line-of-sight geometry.
  If this option is turned on, i.e., the "Pre-calculate line-of-sight geometry" control parameter is set to "t", then the line-of-sight geometry will be calculated before the wavelength loop. Otherwise, the line-of-sight geometry is re-calculated for each wavelength. Both options are identical for a single wavelength. In the case of multiple wavelengths first option is faster but requires much memory consumption.

- High resolution calculations for the refraction.
  If this flag is set to "t" the calculations of the path length of refracted beams will be done at a high vertical resolution assuring the highest possible quality.

- Integration over L-of-S in Fourier space?.
  For the "Integration over L-of-S in Fourier space?" control parameter the setting "yes" is only allowed in the current version.

3.8 Observation and illumination geometries

Appropriate control file: "control_geom.inp"

In this section will be described all control parameters related to the illumination and observation geometry.

3.8.1 Instrument viewing and solar light directions

Relevant control parameters: "Angle selection mode", "Azimuth angles", "Field of view integration", "Field of view size", "Lines of sight number for FOV integration", "Shape of

FOV function", "Solar zenith angles", "Type of LOS definition", "Viewing angles", "Viewing direction",

"Viewing direction" parameter is used to control the viewing direction of the instrument. For space-born instruments as well as for downward looking air- and balloon-borne instruments "Viewing direction" parameter should be set to "dn". In opposite, for ground based measurements as well as for upward looking air- and balloon-borne "Viewing direction" parameter should be set to "up".

"Angle selection mode" parameter defines how the input values for solar zenith angle, viewing angle, and azimuth angle described below have to be handled by the program:

- In "one" mode all three sets of angles are coupled and the line-of-sights are defined sequential by the angle triples, i.e., first line-of-sight is defined by the first value in each angle set, second - by second value and so on. In this case the number of elements in each angle set has to be the same and equal to the desired number of output line-of-sights. For example, if two solar zenith angles (Ψ_1, Ψ_2), two viewing angles (μ_1, μ_2) and two azimuth angles (φ_1, φ_2) are selected, the output will be calculated at two line-of-sights defined by the following angle triplets: $\langle \Psi_1, \mu_1, \varphi_1 \rangle$ and $\langle \Psi_2, \mu_2, \varphi_2 \rangle$.
- In "all" mode all angles are defined independently and output line-of-sight set incorporates all possible combinations of input angles. The number of output line-of-sights in this case is given by the product of the element numbers in each angle set. For example, if two solar zenith angles (Ψ_1, Ψ_2), two viewing angles (μ_1, μ_2) and two azimuth angles (φ_1, φ_2) are selected, the output will be calculated at eight line-of-sights defined by the following angle triplets: $\langle \Psi_1, \mu_1, \varphi_1 \rangle$, $\langle \Psi_2, \mu_1, \varphi_1 \rangle$, $\langle \Psi_1, \mu_2, \varphi_1 \rangle$, $\langle \Psi_2, \mu_2, \varphi_1 \rangle$, $\langle \Psi_1, \mu_1, \varphi_2 \rangle$, $\langle \Psi_2, \mu_1, \varphi_2 \rangle$, $\langle \Psi_1, \mu_2, \varphi_2 \rangle$, and $\langle \Psi_2, \mu_2, \varphi_2 \rangle$.

The number of solar zenith angles, viewing angles, and azimuth angles define the number of elements in the corresponding angle set. All three values have to be the same if "Angle selection mode" is set to "one" (see also limitations below).
Limitation:

- if "RTM-CORE" parameter is set to "ASYMP" (see Section 3.6) only single solar zenith angles, viewing angles, and azimuth angles can be selected.

To define desired values of solar zenith angles and observation line-of-sight angles there are the following options.

- Define solar zenith angles.
  The control parameter "Solar zenith angles" defines the values of the local solar zenith angle (in [deg]) at the observer position. The value of 0° means the sun in zenith, large values of solar zenith angle correspond to twilight conditions (see also limitations below). The input values can be typed either space or comma separated in a row or in a column.
  Attention:
  - If the "RTM Mode" parameter is set to "spher_alb", then in the "Solar zenith angles" control line should be given the number of solar zenith angles rather than their values. The choice of the solar zenith angles grid is done automatically (Gaussian nodes) by the program. The solar zenith angles grid is used by the program to perform integration of the intensity over the solar zenith angles.

  Limitations:

- in plane-parallel mode (see Section 3.4.1) errors are increasing for solar zenith angles larger than $\sim 75°$
- in pseudo-spherical mode (see Section 3.4.3) errors are increasing for solar zenith angles larger than $\sim 92°$
- in spherical mode (see Section 3.4.4) multiple scattering contribution at solar zenith angles larger than $98°$ is set to zero.

- Define zenith viewing angles.
  The control parameter "Type of LOS definition" defines how the input values for "Viewing angles" will be handled by the program. The following modes are available:
  - "th" - the input values are treated as tangent heights in [km]. The value of 0 km correspond to the line-of-sight tangential to the Earth's surface. Tangent heights may also be negative. However, they must not be smaller than minus Earth's radius (see Section 3.4) and larger than top of the atmosphere (see Section 3.3);
    Limitations:
    ◦ This mode is only available if "RTM_TYPE" is set to "spher_scat", i.e., in the spherical atmosphere (see Section 3.4.4).
  - "va" - the input values are treated as viewing angles in [deg]. Selected values must be between $0°$ and $90°$. The value of $0°$ means "nadir" in satellite observation mode ("Viewing direction" is set to "dn") and "zenith" in ground based observation mode ("Viewing direction" is set to "up");
  - "ca" - the same as "va" but the input values are treated as cosines of viewing angles;
  - "au" - the viewing angles will be selected automatically dividing the relevant range of the cosine of the viewing angle [0.01,0.99999] into equidistant intervals. The number of intervals is defined by the second entry of "Type of LOS definition" parameter. The "Angle selection mode" will be set automatically by the program to "all".

  - "ga" - the Gaussian nodes will be used as viewing zenith angle grid. The number of zenith angles is defined by the parameter "Number of streams" (see Section 3.7.4). Settings in control parameter "Viewing angles" will be ignored by the program. The "Angle selection mode" will be set automatically by the program to "all".

  The control parameter "Viewing angles" defines the values of line-of-sight angles (also referenced as viewing angles or zenith angles) as described above. The input values can be typed either space or comma separated in a row or in a column.
  Limitations:
  - limb viewing geometry (line-of-sight does not hit the Earth's surface) is not supported in non-spherical mode (see Section 3.4) .
  - in non-spherical mode errors may be increasing for viewing angles larger than $\sim 30°$ depending on solar zenith angle, viewing direction, observer position, wavelength, etc.

- Define viewing azimuthal angles.
  The control parameter "Azimuth angles" defines the values of the relative azimuth angles of line-of-sight with respect to the sun. The value of $0°$ means the instrument is pointed into the solar direction, and the value of $180°$ means anti-solar direction. Due

to an azimuthal symmetry of the radiative transfer model the values between 180° and 360° define the same observation geometry as the corresponding values between 0° and 180°. The input values can be typed either space or comma separated in a row or in a column.

- Integration over the instrument field of view.
  An integration over the instrument field of view can be performed setting "Field of view integration" control parameter to "t". The field of view size is set in "deg" using the "Field of view size" control line.
  Shape of the field of view function can be select as "Boxcar" or "Gaussian", setting in the "Shape of FOV function" control line "1", or "2", respectively.
  The number of lines of sight to perform numerical integration over the field of view needs to be specified in the "Lines of sight number for FOV integration" control line (must be an odd integer greater or equal to 3).
  Limitations:
  - In the discrete ordinate mode ("RTM-CORE" parameter is set to "DOM_S" or "DOM_V", see Section 3.6) the field of view integration is only supported for a spherical atmosphere (see Section 3.4).
  - Gaussian field of view function is supported only in CDI mode.

3.8.2 Observer position

Relevant control parameters: "Position of the instrument", "User-defined output altitude"

The observer position is defined in "Position of the instrument" input line. There are the following options:

- "toa" or "boa"
  - the instrument is supposed to be located at the top of the atmosphere or at the surface;
- "too" or "boo"
  - the instrument is supposed to be located at the top or at the bottom of the ocean (relevant for coupled ocean-atmosphere mode only);
- "sagl" or "user"
  - the instrument position in the atmosphere, above the atmosphere or in the ocean can be specified by user.
  The corresponding altitude values are defined setting parameter "User-defined output altitude" to desired altitudes in [km] for atmosphere and to desired depths in [m] for ocean.
  Attention:
  - multiple user-defined output altitudes is allowed if "RTM Mode" parameter set to "int" only (see Section 3.1.1);
  - only single user-defined output altitude is allowed if it is above TOA or control parameter "RTM_TYPE" is set to "spher_scat";
  - selected altitude must be positive for the atmosphere and negative for the ocean;
  - user-defined output altitudes have to be monotonically increase or decrease;
  - the option "user" requires more computation time as compared with the option "sagl", it is recommended to use option "user" if the altitude of instrument position does not coincide with a level of main altitude grid (Section 3.3);

- if the mode "sagl" is chosen the altitude of instrument position will be shifted by the program to the nearest main altitude grid (see Section 3.3).

If the mode "user" is chosen the altitude of instrument position is equal to given in "User-defined output altitude" input line. The implemented in SCIATRAN code technique does not require interpolation and provides an exact value of the intensity/Stokes vector using the analytical representation of the solution within a layer.

Limitation:

- the instrument position can be defined either in the atmosphere, or in the ocean;
- the mode "user" can not be used if "Single scattering correction" parameter is set to "t" (see Section 3.7.5) or inelastic processes within water (VRS and/or fluorescence) should be accounted for (see Section 3.20).

3.9 Spectral intervals/windows and wavelength grid

Appropriate control file: "control.inp"
Relevant control parameter: "Spectral segment info"

Generally, any spectral interval/window between 175.44 nm and 40 micrometers can be selected. However, aerosols can only be switched on at wavelengths longer than 240 nm (see Section 3.14.1). Furthermore, correlated-k parameters (see Section 3.10.4) are pre-calculated only in sub-intervals related to the GOME/SCIAMACHY spectral channels, i.e., 240-1750 nm (channels 1-6), 1940-2040 nm (channel 7), and 2260-2385 nm (channel 8).

Selection of more than one spectral intervals is also allowed. There should be no overlap between spectral intervals and they have to be ordered by wavelength.
The number of spectral windows is defined by the first entry in the first line of "Spectral segment info" control field. The second entry of the first line this control field defines the units of the spectral grid ('nm' for wavelength or 'cm-1' for wavenumber). The input spectral information is then read by the program from lines below starting from the second line in "Spectral segment info" control field. The number of control lines which will be read is defined by the number of spectral windows selected by user. Any other lines below are ignored. Interpretation of the control lines starting from the second one depends on the first entry in the particular line which can be set to "1" or "2":

- "1" - the values from the second to the fourth in the line will be interpreted as start wavelength, number of required wavelengths, and stepsize, respectively;
- "2" - the values from the second to the fourth in the line will be interpreted as start wavelength, end wavelength, and stepsize, respectively.

The first entry may be different for different spectral windows. For example, the input field below

```
Spectral segment info
2, nm
1, 324.6, 10, 0.2
2, 354.6, 355.7, 0.1
```

can be used to define following two spectral windows: the first from 324.6 nm to 326.4 nm containing 10 equidistant spectral points with an increment of 0.2 nm and the second from 354.6 nm to 355.7 nm containing 12 equidistant spectral points with an increment of 0.1 nm.

Alternatively, a wavelength grid can be read from a file. Setting the first entry in the "Wavelength grid from file" input line to "t", the second entry specifies the name of the file containing the wavelengths grid [nm] and the third entry defines the column number to be read.
Attention:

- The wavelength grid from the file will be used instead of the equidistant grid specified in the "Spectral segment info" control field. However, the number of the spectral channels as well as start and end wavelengths for each spectral channel are kept as specified in the "Spectral segment info" control field.
- If the "ESFT" mode (see Sections 3.10.2 and 3.10.4) is switched on and the convolution is switched off (see Section 3.11) the output wavelength grid will be automatically changed by the program to match the internal wavelength grid appropriate to the ESFT data base (see Section 3.10.4).
- In the retrieval mode (see Sec. 3.1.9) the wavelength grid from the measurement data file is used for the forward modeling. Thus only the information on spectral segments (i.e., start and end wavelengths) will be kept from the input in the "Spectral segment info" control field.

3.10 Atmospheric trace gases - spectral information

Appropriate control file: "control.inp"
Relevant control parameter: "Forward model: trace gases"

The following atmospheric trace gases implemented in the current version of SCIATRAN: O_3, NO_2, ClO, OClO, BrO, HCHO, SO_2, NO_3, O_4, O_2, H_2O, CO_2, CO, CH_4, N_2O, NO, NH_3, HNO_3, OH, HF, HCL, HBR, and HI.

Due to a different treatment of spectral information one should distinguish between so-called "line-absorbers", such as e.g., H_2O, CO_2, CO, CH_4, and N_2O, which feature complex absorption bands strongly dependent on pressure and temperature and ordinary "continuum-absorbers", such as O_3, NO_2, ClO, OClO, BrO, HCHO, SO_2, NO_3, O_4. A special treatment is needed for O_2 which is considered as a "continuum-absorber" in UV spectral region and as a "line-absorber" in Vis-NIR spectral region.
Attention:
The absorption coefficients of O_3, NO_2, SO_2, ClO, and HCHO are calculated by program using the cross sections in the UV-Vis spectral range and HITRAN line parameters in the IR spectral range. The control line "Longest wavelength for cross sections" in the control file "control_la.inp" defines for these species the longest wavelengths of the cross sections treatment, i.e., at all wavelengths shorter than or equal to the specified wavelength the cross sections are used whereas at longer wavelength the absorption coefficients are calculated using the spectral parameters from the HITRAN database (LBL or ESFT).
This setting is intended for developing only and should not be changed by ordinary users.

A contribution of a particular trace gas into the total absorption can be switched on or off

setting an appropriate flag in the "Forward model: trace gases" input line. The following options are relevant:

- list of trace gase names to be included in the forward model (separated with comma or space);
- 'all' $\longrightarrow$ turns on all trace gases;
- 'none' $\longrightarrow$ turns off all trace gases.

Attention:
An absorber can be automatically switch off by the program if within selected windows there is no absorption of this trace gas.

3.10.1 Cross sections

Appropriate control files: ""control.inp", "xsections.inp"
Relevant control parameters: "X-section path", "X-sections settings input file", all keywords in "xsections.inp" file

The contribution of "continuum-absorbers" into the total absorption coefficient at a particular temperature is obtained using a set of cross-sections measured in the laboratory at different temperatures. In the present version of SCIATRAN cross-sections are assumed to be independent of pressure.

- General.
  The path to the cross section data base should be specified in "X-section path" input field. All parameters needed to select appropriate cross sections for "continuum-absorbers" are contained in "xsections.inp" file. The contents of this file are discussed below.

  Parameter "Do x-sections akima interpolation" is used to control if trace gas cross sections will be interpolated linearly (setting "f") or a cubic interpolation as described in (Akima, 1970) (setting "t") will be employed instead.

  Cross sections of all "continuum-absorbers" are specified in "xsections.inp" file using a standard input field described below.
  - The first line of the input field contains a keyword consisting of a common mark, "X-section:", and a label defining which trace gas the cross sections belong to.
  - The second line contains a value defining the number of cross sections of the particular trace gas measured at different temperatures.
  - Each subsequent line starting from the third one contains a file name for a particular cross section and an appropriate temperature. The number of lines which will be read by the program starting from the third one is defined by the number of cross sections specified by user in the second line. All lines below will be ignored.

  Attention:
  cross sections need not to be specified for trace gases switched off in "Forward model: trace gases" control lines.

- O_2 Schumann-Runge and Herzberg absorption bands.
  Two separate inputs are needed to describe O_2 absorption structure in Schumann-Runge (175.43 - 204.08 nm) and Herzberg (190 - 240 nm) bands. They are marked as

"X-section: o2 UV" and "X-section: o2 Herzberg", respectively.
Attention:
at present, temperature parameterization is available in Schumann-Runge absorption band only.

- O_3 absorption bands.
  To obtain the ozone cross section in the entire spectral range covered by the program two cross section parts are joined. The standard cross section defined in "X-section: o3 UV-NIR" input field which is valid in UV-Vis-NIR spectral range at wavelengths longer than 240 nm is extended employing a cross section defined in "X-section: o3 ¡ 240 nm" input field. A discontinuity may occur at a joint point.

  Due to a strong temperature dependence of ozone absorption in UV spectral region a temperature parameterization is commonly used instead of cross sections measured at discrete temperatures. A type of temperature parameterization can be selected between GOME FM (Burrows et al., 1998, 1999) and Bass-Paur (Paur and Bass, 1984) by means of appropriate setting of "Do O3 UV GOME FM" parameter. According to the selected parameterization mode a name of the file containing temperature parameters should be specified in "X-section: o3_uv, GOME FM" or "X-section: o3_uv, Bass" followed by the start and end wavelength in [nm], defining the spectral interval where the ozone cross section defined in "X-section: o3 UV-NIR" will be replaced by the selected temperature parameterization. Only one line below the keyword is meaningful. Setting made for inactive parameterization have no effect.
  Attention:
  - There is no temperature parameterization available below 240 nm.
  - A discontinuity may occur at joint points.

- O_4 absorption bands.
  Attention: Please take into account that data values in the input file containing O_4 cross-section should be presented in [$cm^5\,molecule^{-2}$] and multiplied by 10^{+40}.

3.10.2 Treatment of "line-absorbers"

Appropriate control file: "control.inp", "control_la.inp"
Relevant control parameters: "Line absorber treatment", "Line absorber windows", "Spectral windows for line absorbers"

The "line-absorbers" are taken into account calculating an absorption contribution at a particular wavelengths, pressure and temperature based on a set of spectroscopic parameters, such as line position, line intensity, air-broadened half-width, etc., obtained from the HITRAN 2000 spectroscopic data base (Rothman et al., 2003). The following program modes selected by setting "Line absorber treatment" parameter to a desired keyword are implemented in order to accurately consider "line-absorbers":

- "lbl" - an accurate line-by-line computation, additional settings needed in the line-by-line mode are described in Section 3.10.3;
- "esft" - a significantly faster correlated-k (c-k) approximation which is also referenced to as the exponential sum fitting (ESFT) approach (see (Buchwitz et al., 1998, 1999, 2000) for details), additional settings needed in the esft mode are described in Section 3.10.4;

- "off" - turns treatment of all "line-absorbers" off independent of settings made in "Forward model: trace gases" control line.

Due to a strong spectral variability of the absorption features of "line-absorbers" a quite small wavelength step should be selected in "Spectral segment info" input field (see Section 3.9) to get a reasonable accuracy, values of the order of 0.001 nm or even smaller are recommended. For a practical use spectra calculated in the line-by-line mode should be convolved with an instrument slit function (see Section 3.11).

Changing "Line absorber windows" parameter user can control if the "line-absorbers" contribution is considered in the entire spectral interval selected by user (see Section 3.9) or in specific subintervals only. For example, setting this option to "t" one can save a lot of time if you are intending to perform calculations in a wide spectral interval containing only a relatively narrow absorption band of a "line-absorber". In the line-by-line mode, however, this option can be only used if convolution is switched on (see Section 3.11).

If "Line absorber windows" parameter is set to "t" the "line-absorbers" contribution will be considered only within spectral subintervals specified in "Spectral windows for line absorbers" input field. The value in the first line defines the number of spectral subintervals to be used and the subsequent lines contain start and end wavelength of the particular subinterval in [nm]. The number of lines read by the program starting from the second one is equal to the number of spectral subintervals specified by user in the first line, all lines below will be ignored.

3.10.3 Line-by-line mode

Appropriate control file: "control.inp", "control_la.inp"
Relevant control parameters:
"Line absorber treatment", "Line wing cut-off wavenumber"

Line-by-line mode is selected if "Line absorber treatment" parameter is set to "lbl" (in the "control.inp" file). In this mode an additional path to the HITRAN database files need to be set in input field "Path to the line parameter database". The filename need not to be changed unless you explicitly want to use another database.

To obtain a contribution by a particular trace gas in the total absorption in the line-by-line mode a summation of contributions due to individual absorption lines of the trace gas is performed. Parameter "Line wing cut-off wavenumber" defined in cm^{-1} is used to control the contribution range, i.e., at a particular wavelength only absorption lines having their central wavelength within a distance specified by "Line wing cut-off wavenumber" parameter are considered. The contribution of all other lines is set to zero.

3.10.4 ESFT mode

Appropriate control files: "control.inp", "control_la.inp", "esft.inp"
Relevant control parameters: "Line absorber treatment", "Path to ESFT data base",
"Do esft anti correlation"

Table 3.1: Spectral coverage of the ESFT data base

Channel	Spectral range, nm	$\Delta\lambda^{c-k}$, nm	"line-absorbers"
1	240 - 405	no absorption features present	
3, 4, and 5	394 - 1070	0.05	H_2O, O_2
6	1070 - 1800	0.2	H_2O, CO_2, O_2, CH_4
7	1920 - 2060	0.025	CO_2, H_2O
8	2230 - 2340	0.025	CH_4, CO, H_2O, N_2O

ESFT mode is selected if "Line absorber treatment" parameter is set to "esft" (in the "control.inp" file). In this mode an additional path to the ESFT data base should by specified in "Path to ESFT data base" input field in the "control_la.inp" control file.

ESFT data base was generated only in sub-intervals related to the GOME/SCIAMACHY spectral channels. The spectral channels along with appropriate averaging intervals, $\Delta\lambda^{c-k}$, which were used to generate the ESFT data base are listed in Table 3.1. The averaging interval is related to the spectral resolution of SCIAMACHY instrument and is specific for each particular channel.

Please note, spectral intervals between channels 6 and 7 (1800 - 1920 nm) as well as between channels 7 and 8 (2060 - 2230 nm) of the SCIAMACHY instrument are **not covered** by the ESFT data base.

Attention :

- If convolution is switched off (see Section 3.11) the output wavelength grid will be automatically changed by the program to match the internal wavelength grid appropriate to the ESFT data base. The reason is that in the ESFT mode each particular wavelength selected for the radiative transfer calculation has to be identical with the center wavelength of the ESFT spectral pixels contained in the data base. For example, 760.025 nm is the center wavelength of pixel 760.000 nm - 760.050 nm lying in the oxygen A-band, where the wavelength is sampled every 0.05 nm. The next spectral point, therefore, is 760.025 nm + 0.05 nm = 760.075 nm, and so on. Thus, if you select, for example, an input wavelength of 760.04 nm it will be shifted by the program to the nearest spectral point appropriate to ESFT data base, i.e., to 760.025 nm.
- A detailed set of input parameters needed to read and process information from the ESFT data base is contained in "esft.inp" control file. This file should not to be changed by user.
- Parameter "Do esft anti correlation" must always be set to "f". Setting "t" is only used by experts to create or to update ESFT data bases.

3.11 Convolution

Appropriate control file: "control.inp", "control_conv.inp"
Relevant control parameters: "Do convolution", "Convolution for line absorber only", "Slit function type", "Slit function HWHM", "Slit function wing cut-off",
"Slit function filename", "Internal wavelength step"

The "Do convolution" parameter ("control.inp" file) is used to control if convolution needs to be performed. If convolution is switched on an internal wavelength grid will be created to perform the radiative transfer calculations. After the convolution the spectra will be written out on the original wavelength grid as selected in "Spectral segment info" input field ("control.inp" file) (see Section 3.9).
In the ESFT mode (see Section 3.10.4) the step of the internal wavelength grid is read from the ESFT data base, otherwise the value specified in the "Internal wavelength step" input line [nm] is used.
Attention :

- To get a reasonable accuracy in line-by-line mode a quite small wavelength step (0.001 nm or even smaller) is recommended (see Section 3.10.2).

If "Convolution for line absorber only" parameter is set to "t" convolution is not performed at spectral points where "line-absorbers" does not contribute into the total absorption. If "Line absorber windows" parameter is set to "t" these are the spectral points locating outside the spectral intervals specified in "Spectral windows for line absorbers" input field (see Section 3.10.2). In the ESFT mode (see Section 3.10.4) the spectral points which are not present in the ESFT data base are also excluded from the convolution.

The instrument slit function should be defined in the control line "Slit function type". The entry can be at present "1", "2", "3":
"1" - Gaussian slit function;
"2" - boxcar slit function;
"3" - user-defined slit function.

If the "Slit function type" parameter is set to "1" (Gaussian), then the following parameters need to be specified:

- "Slit function HWHM" - slit function half width at half maximum in nm, needs to be specified for each spectral interval selected in "Spectral segment info" input field (see Section 3.9);
- "Slit function wing cut-off" - slit function wing cut-off defining the convolution range in numbers of HWHM, i.e., only spectral points located closer to the central wavelength than the selected distance contribute into the result.

If the "Slit function type" parameter is set to "3" (user-defined) then "Slit function filename" control parameter should be defined. In this control field the slit function for each spectral segment is to be specified. The number of conrol lines has to be equal to the number of spectral segments selected in the "control.inp" file. The first entry in each control line specifies the wavelength for which the slit function is supplied (central wavelength). If first entry set to "auto" the central wavelength will be associated to the middle of the spectral range where the slit function is defined. The second entry specifies the slit function filename. The file must contain the wavelength in [nm] in the first column and slit function values in the second

column. The wavelength grid must be monotonously increasing. The slit function is supposed to be the same for all spectral points within a spectral segment.

3.12 Atmospheric trace gases, pressure, and temperature profiles

Appropriate control file: "control.inp", "control_prof.inp"

3.12.1 Standard settings

Relevant control parameters: "Standard profile scenario file name", "Standard profile scenario for line absorbers"

Select vertical profiles of "continuum-absorbers", pressure, and temperature

Parameter "Standard profile scenario file name" defines the path ("/DATA_BASES/PROFILES/B2D/UV-Vis/") and the name of the file containing vertical distributions of "continuum-absorbers" (O_3, NO_2, SO_2, ClO, BrO, NO_3, HCHO, and OClO), see Section 3.10, as well as vertical profiles of pressure and temperature. The vertical distribution for O_4 is calculated from the air density profile.
By default, the SCIATRAN software package incorporates a climatological database obtained from a 2D chemical transport model developed at the University of Bremen Sinnhuber et al. (2009) which is similar to the well-known SLIMCAT model Chipperfield (1999). This database contains monthly and zonally averaged distributions of atmospheric trace gases which show significant adsorbtion features in the UV-Vis-IR spectral range (O_3, NO_2, SO_2, ClO, HCHO, BrO, NO_3, OClO). Additionally, pressure and temperature information is contained. The data is provided in the altitude range 1 - 95 km for 10° latitude bins.
The corresponding filenames usually have the following structure: "mon{xx}lat{yy}{z}.b2d", where "{xx}" denotes the number of the month (01 = January, 02 = February, ..., 12 = December), "{yy}" denotes the latitude band (05 = 0 – 10 deg, 15 = 10 – 20 deg, ..., 85 = 80 – 90 deg), and "{z}" denotes the hemisphere (n = Northern Hemisphere, s = Southern Hemisphere).
Attention :

- If the top of atmosphere height is set to a value higher than 95 km (see Section 3.3) an extrapolation by a constant value of volume mixing ratio will be performed for trace gas vertical profiles.
- Vertical profiles of the temperature and of the logarithm of pressure are extrapolated linearly.

Alternatively, following climatology are available:

- a climatological data base obtained using a 2D chemo-dynamical model developed at MPI Mainz (Brühl and Crutzen, 1993) is employed in SCIATRAN. This data base contains monthly and latitudinal dependent vertical distributions of atmospheric trace gas volume mixing ratios, pressure, and temperature in the altitude region between 0 and 60 km. The filenames appropriate to MPI climatology have the same structure as for B2D climatology files: "mon{xx}lat{yy}{z}.mpi";

- the McLinden climatology (C. McLinden, Meteorological Service of Canada, privat communication) containing monthly and latitudinal dependent vertical distributions of O_3, NO_2, BrO, and OClO volume mixing ratios, as well as pressure and temperature in the altitude region between 0 and 100 km. The filenames appropriate to McLinden climatology have the same structure as for MPI climatology files: "mon{xx}lat{yy}{z}.mcl";
- the US Standard atmosphere (NASA, 1976) containing zonally and seasonally averaged vertical distributions of O_3, NO_2, SO_2, and ClO volume mixing ratios, as well as pressure and temperature in the altitude region between 0 and 120 km can be used. The US Standard atmosphere is represented by "uss76.dat" file.

Atmospheric trace gases switched on in "Forward model: trace gases" control line (see Section 3.10) which are not included in the above discussed data bases will be taken into account in radiative transfer calculations with vertical distributions set to zero.

Select vertical profiles of "line-absorbers", pressure, and temperature

The control parameter "Standard profile scenario for line absorbers" defines the path ("/DATA_BASES/PRO and the name of the file containing vertical distributions of "line-absorbers": H_2O, CO_2, N_2O, CO, CH_4, O_2, NO, NH_3, HNO_3, OH, HF, HCl, Br, HI.

Alternatively, the US Standard atmosphere containing zonally and seasonally averaged volume mixing ratio distributions in the altitude region between 0 and 120 km is available for "line-absorbers" such as (O_2, H_2O, CO_2, N_2O, CO, CH_4), see Section 3.10. Corresponding profiles are stored in "usstandard.dat" file.

3.12.2 Advanced settings

Appropriate control file: "control.inp", "control_prof.inp"

The settings described in this section should be performed if the parameter "Advanced profile settings" in the "control.inp" file is set to "t". If the parameter "Advanced profile settings" is set to "f" the default setting will be performed by the program automatically.

3.12.2.1 Interpolation type

Relevant control parameters:
"Do profiles akima interpolation" (defailt "f")

The control parameter "Do profiles akima interpolation" controls if vertical distributions of atmospheric trace gases as well as vertical profiles of pressure and temperature will be interpolated linearly (setting "f") or a cubic interpolation as described in (Akima, 1970) (setting "t") will be employed instead.

3.12.2.2 Replacements of standard settings

Relevant control parameters:
"Do P and T from standard profile file" (default "t")

"Pressure and temperature file name",
"Trace gas replacement profiles" (default "0")

Replace vertical profile of pressure, and temperature

The standard profiles for pressure, temperature and atmospheric trace gases read from the data base as discussed in Section 3.12.1 can be replaced by the user-defined profiles.
The replacement of vertical profiles of pressure and temperature is performed if "Do P and T from standard profile file" is set to "f". The replacement profiles are read from the file specified in "Pressure and temperature file name" control line. The file name must be followed by the numbers of data columns in the file containing altitude grid, pressure and temperature, respectively. For example, an input line

```
'mon08lat45s.mpi', 2, 3, 4
```

means that the second column in "mon08lat45s.mpi" will be interpreted as altitude in km, the third column is supposed to contain a pressure in mb and the fourth column is considered as a temperature in K. Contents of other columns in the file will be ignored.

Replace vertical profile of trace gases

Replacement of atmospheric trace gas vertical profiles is controlled by "Trace gas replacement profiles" input field. The first line in this control field specifies how many replacement profiles will be supplied, setting this value to "0" means that no replacement will be performed. The subsequent lines must include the file name containing the replacement profile, name of the trace gas which the replacement profile belong to (e.g.,"O3"), units of the replacement profile ("conc" or "vmr"), as well as the numbers of data columns in the file containing altitude grid and the trace gas vertical profile. The number of input lines read by the program starting from the second one is equal to the number of replacement profiles specified by user in the first input line. Any lines below will be ignored. For example, an input

```
2
'conc_const.o3', 'O3', 'conc', 1, 2
'mon07lat45n.mpi', 'NO2', 'vmr', 2, 6
'mon08lat45n.mcl', 'BrO', 'vmr', 2, 9
```

means that the vertical distributions of O_3 and NO_2 will be replaced, no replacement will be done for BrO. The first data column in the file "conc_const.o3" is supposed to contain the altitude grid appropriate to the replacement profile of O_3 contained in the second data column. The replacement profile is expected to be supplied as a vertical distribution of O_3 number density in mol/cm^{-3}. Similarly, the second data column of "mon07lat45n.mpi" is supposed to contain the altitude grid appropriate to the replacement profile of NO_2 contained in the sixth data column. The replacement profile is expected to be supplied as a vertical distribution of NO_2 volume mixing ratio in ppmv.

Attention :

- Vertical distributions of atmospheric trace gases not contained in the standard climatology (see Section 3.12.1), i.e., having zero amounts by default, can also be replaced.
- If an appropriate replacement is specified, vertical profiles of O_3 and temperature read from an ozone climatology, see Section 3.12.2.4, are replaced as well.

3.12.2.3 Scaling of O_3, H_2O, N_2O, and pressure vertical profiles

Relevant control parameters:
"Ozone profile scaling" (defailt "f"),
"Water vapor profile scaling" (defailt "f"),
"NO2 profile scaling" (defailt "f"),
"Pressure profile scaling" (defailt "f")

The vertical profiles of O_3, H_2O, and N_2O can be scaled to matched the desired value of they vertical columns. If the first entry in the "Ozone profile scaling", "Water vapor profile scaling" or "NO2 profile scaling" input lines is set to "t" than second entry will be used by the program as desired vertical column of O_3 in [DU], H_2O in [gr/cm^2], and N_2O in [molecule/cm^2], respectively.
If the first entry in the "Pressure profile scaling" input line is set to "t" than the second entry will be used by the program as the surface pressure. The existing pressure profile will be scaled to have a given surface pressure.

3.12.2.4 Ozone and BrO climatologies

Relevant control parameters:
"Ozone climatology" (defailt "NONE"),
"Path to ozone climatology", "Scale climatological profile", "Ozone total column",
"BrO climatology" (defailt "f"),
"BrO climatology file"

Set ozone climatology
Ozone climatologies can be used setting the "Ozone climatology" control parameter to any supported value other then "NONE". An appropriate path to the ozone climatology data base should be specified in "Path to ozone climatology" control line. Once the ozone climatology is switched on, the vertical profiles of ozone and temperature from the standard data bases (see Section 3.12.1) will be replaced by the climatological values. The following entries are valid for "Ozone climatology" parameter:

- "IUP_BREMEN" - a climatology developed at Institute or Environmental Physics/Institute of Remote Sensing (University of Bremen) based on ozonesonde and satellite data (Lamsal et al., 2004). The climatology contains ozone column classified parameterization of ozone and temperature vertical profiles for 4 seasons ordered by the day of year (0 – 120, 121 – 181, 182 – 304, 305 – end of year) , and 9 latitude bands (90°S – 65°S, 65°S – 55°S, 55°S – 35°S, 35°S – 25°S, 25°S – 25°N, 25°N – 35°N, 35°N – 55°N, 55°N – 65°N, 65°N – 90°N; the upper, i.e., high latitude, boundary of each interval is always associated to the next latitude interval).
- "TOMS_V7" - version 7 of a climatology developed by NASA based on the measurements of ozone vertical distribution performed by the TOMS instrument (Wellenmeyer et al., 1997). The climatology contains ozone column classified parameterization of ozone and temperature vertical profiles for 9 latitude bands (same as for "IUP_BREMEN" climatology).
- "TOMS_V8" - version 8 of a climatology developed by NASA based on the measurements of ozone vertical distribution performed by the TOMS instrument. The climatology

comprises monthly data sets for 18 latitude bands of 10° width containing temperature vertical profiles and a parameterization of ozone vertical distribution classified by the ozone total column.

- "TOMS_M" - a climatology developed by NASA based on the measurements of ozone vertical distribution performed by the TOMS instrument. The climatology comprises monthly data sets containing ozone and temperature vertical profiles for 18 latitude bands of 10° width. No classification by the ozone total column is available.
- "KNMI" - a climatology developed at the Royal Netherlands Meteorological Institute (KNMI) based on ozonesonde and satellite measurements (Fortuin and Kelder, 1998). The climatology comprises monthly data sets containing ozone and temperature vertical profiles for 17 latitude bands of 10° width between 85°S and 85°N. No classification by the ozone total column is available.
- "UGAMP" - a climatology developed at the University of Reading[1] consists of a 4-dimensional distribution of ozone that has been built up from the combination of several observational data sets. The data sets include satellite observations (SBUV, SAGE II, SME, TOMS) as well as ozone sonde data provided by the Atmospheric Environment Service of Canada averaged over 5 years (1985 to 1989). The climatology comprises monthly data sets of ozone vertical distribution with a horizontal resolution is of 2.5 by 2.5 degrees (144 points in longitude and 73 points in latitude from pole to pole).

The control parameter "Ozone total column" defines the value of total ozone in DU which is used to obtain an appropriate vertical profile for ozone if "Ozone climatology" parameter is set to "IUP_BREMEN", "TOMS_V7", or "TOMS_V8" as well as an appropriate vertical profile for temperature if "Ozone climatology" parameter is set to "IUP_BREMEN" or "TOMS_V7". If "Ozone climatology" control parameter is set to "TOMS_M" or "KNMI", ozone vertical distribution extracted from the selected climatological data base can be scaled to obtain a desired total column of ozone setting "Scale climatological profile" parameter to "t". Setting of "Scale climatological profile" parameter has no effect for "IUP_BREMEN", "TOMS_V7", "TOMS_V8", and "UGAMP" climatologies.

Attention:

- Latitude must be set as described in Section 3.18.
- If "Ozone climatology" parameter is set to "IUP_BREMEN", "TOMS_V8", "TOMS_M", "KNMI", or "UGAMP", the date must be set as described in Section 3.18.
- If an appropriate replacement is activated as described in Section 3.12.1, the climatological profiles of both ozone and temperature will be re-replaced.

Set BrO climatology

The BrO climatology can be used setting the "BrO climatology" control parameter to "t". An appropriate path to the BrO climatology data base should be specified in "BrO climatology file" control line. The current version of SCIATRAN allows to use the BrO climatology from MIPAS CFC-11 measurements. Once the BrO climatology is switched on, the vertical profiles of BrO from the standard data bases (see Section 3.12.1) will be replaced by the climatological values.

[1] http://badc.nerc.ac.uk/data/ugamp-o3-climatology/

3.12.2.5 Photochemically active species

Appropriate control file: "control.inp", "control_pas.inp"
Relevant control parameters: "Altitude grids for photochemically active species", "Number of photochemically active species", "Photochemical calculations", "Profiles for photochemically active species", "Replace tropospheric concentrations", "Trace gas selection - photochemistry", "Tropopause height", "Solar zenith angle for constant profile", "Use constant profile"

Setting "Photochemical calculations" parameter to "t" photochemically active species can be considered in the radiative transfer calculations. For these species solar zenith angle dependent vertical distributions will be used in radiative transfer model instead of fixed (solar zenith angle independent) vertical profiles. Total number of photochemically active species to be considered by the program is controlled by "Number of photochemically active species" parameter. The names of atmospheric trace gases which will be considered as photochemically active are specified in "Trace gas selection - photochemistry" input line, the names must be separated by space or comma. The number of names read by the program is equal to the total number of photochemically active species defined by user in "Number of photochemically active species" control line. Any other gas names in the list will be ignored.

For each photochemically active species a file containing an altitude grid and a file containing a set of vertical distributions for different solar zenith angles must be specified in "Altitude grids for photochemically active species" and "Profiles for photochemically active species" input fields, respectively. The altitude grid file should contain one column of altitude grid levels. The first column of the profile file should contain values of solar zenith angle and all other columns contain the number densities at different altitude level, i.e., each line of the profile file must contain a vertical distribution of the corresponding trace gas appropriate to the solar zenith angle defined by the first value in this line. The number of input lines in both "Altitude grids for photochemically active species" and "Profiles for photochemically active species" control fields read by the program is equal to the total number of photochemically active species defined by user in "Number of photochemically active species" control line. Any lines below will be ignored.

Please note, photochemical data base is not a part of SCIATRAN, solar zenith angle dependent vertical distributions mentioned in this section have to be provided by user.

Since most of photochemical models are not valid in the troposphere, an unrealistic information obtained from a model for a particular trace gas in this altitude region can be replaced by a fixed, i.e., solar zenith angle independent, vertical distribution for this trace gas setting a corresponding flag in "Replace tropospheric concentrations" control line to "t". In this case the values from the standard (non-photochemical) profile (Sections 3.12.1 and 3.12.2.2) will be used below the tropopause rather than values predicted by a photochemical model. The number of logical flags read by the program in "Replace tropospheric concentrations" control line is equal to the total number of photochemically active species defined by user in "Number of photochemically active species" control line. Any other flags in the list will be ignored.

The tropopause height in [km] is defined in "Tropopause height" control line. Only one value is accepted in this control line, i.e., the tropopause height is the same for all photochemically

active species. Setting of the "Tropopause height" control parameter has no effect if all entries in ''Replace tropospheric concentrations" control line are set to "f".

If any flag in the "Use constant profile" control line is set to "t" the solar zenith angle dependent vertical distribution of the corresponding photochemically active species will be replaced by a fixed vertical profile from the same photochemical data base appropriate to the solar zenith angle specified in "Solar zenith angle for constant profile" input line. If necessary, an interpolation is performed. The number of logical flags read by the program in "Use constant profile" control line is equal to the total number of photochemically active species defined by user in "Number of photochemically active species" control line. Any other flags in the list will be ignored. Only one value is accepted in "Solar zenith angle for constant profile" control line, i.e., fixed profiles for all photochemically active species are selected at the same solar zenith angle. Setting of the "Solar zenith angle for constant profile" control parameter has no effect if all entries in "Use constant profile" control line are set to "f".
Limitation:

- The photochemical calculations can only be performed in "CDI" mode (see Section 3.6).

3.13 Rayleigh scattering

Appropriate control files: "control.inp" and "control_ray.inp"
Relevant control parameters: "Advanced Rayleigh settings"

All parameters needed to calculate the Rayleigh scattering in the atmosphere can be installed using default setup. Setting the "Advanced Rayleigh settings" parameter to "f", the default mode is switched on (see Section 3.13.1). Otherwise ("t") the Rayleigh scattering parameters should be adjusted by user in the file "control_ray.inp" (see Section 3.13.2).

3.13.1 Default settings

To use this option the user must set in the "Advanced Rayleigh settings" input line "f" ("control.inp"). If the default setup is chosen the Rayleigh scattering coefficient and the King factor is calculated according to Bates approach (Bates, 1984). The user can not look in the file "control_ray.inp" in this case at all.
Attention:
The Rayleigh scattering phase matrix (function) includes automatically the anisotropy effects according to the Bates approximation.

3.13.2 Advanced settings

If "Advanced Rayleigh settings" is set to "t" the adjustment of some parameters in the file "control_ray.inp" is required. The following options are available:

- Scaling of Rayleigh scattering coefficient.
  If the first entry in the "Rayleigh scattering scaling" input line is set to "t", then the second entry will be interpreted by the program as a scaling factor. The Rayleigh scattering coefficient will be *multiplied* by this scaling factor at all wavelengths.

- Setting the Rayleigh optical thickness manually.
  If the first entry in the "Rayleigh optical thickness" input line is set to "t", then the second entry will be interpreted by program as a desired Rayleigh optical thickness. This option allows, for example, to eliminate impact of different Rayleigh cross-section approximations and numerical integration rules comparing SCIATRAN results to benchmark results or other codes.
  Attention: The Rayleigh optical thickness is independent of the wavelength if this option is used.

- Create file containing Rayleigh cross-section and optical thickness at selected wavelengths.
  First line after "Wavelength grid for Rayleigh scattering output" input parameter defines the wavelength grid at which information about Rayleigh scattering will be put into the output file named "SCE_RAYLEIGH.OUT". This output file together with all other output files are stored in the directory "./DATA_OUT".
- Select formula for the Rayleigh cross-section calculation.
  Setting 1, 2, 3, or 4 in the "Rayleigh scattering index" input line, the user can select different approaches to calculate the Rayleigh sross-section, i.e.,:
  "1" - according to Bates (as by default mode);
  Limitation: It can be used in the spectral range $[0.2 - 30]\,\mu$m.
  "2" - according to (Bucholtz, 1995) with the refractive index from (Peck and Reeder, 1972) and effective King factor for air from (Bates, 1984);
  Limitation: It is recommended to use in the spectral range $[0.2 - 4.0]\,\mu$m.
  "3" - according to (Bodhaine et al., 1999) with the refractive index from (Peck and Reeder, 1972) and weighted King factor which includes contribution of N_2, O_2, Ar, and CO_2;
  Limitation: It is recommended to use in the spectral range $[0.25 - 1.0]\,\mu$m.
  "4" - user defined (see below).
- Set volume concentration of N_2, O_2, Ar, and CO_2.
  The four entries in the "Percent volume concentration" input line define relative concentrations of N_2, O_2, Ar, and CO_2 which will be used for calculation of King factor.

If "Rayleigh scattering index" is set to "4" (user defined mode) the additional setting of parameters have to be done in the file "control_ray.inp" to calculate the Rayleigh scattering coefficient:

- Set Lorentz-Lorenz factor in the Rayleigh scattering cross-section.
  Setting in the "Lorentz-Lorenz factor" input line "a", "b" or "c", the user can switch between three Lorentz-Lorenz factors which should be used in the Rayleigh cross-section formula (below n is the refractive index of air):
  "a" - $(n^2 - 1)/(n^2 + 2)$, i.e., without approximations;
  "b" - $2/3(n - 1)$, i.e., $n + 1 \approx 2$; $n^2 + 2 \approx 3$
  "c" - $1/3(n^2 - 1)$, i.e., $n^2 + 2 \approx 3$

- Set refractive index of air.
  User can set the desired value of the air refractive index putting in the "Refractive index" input line "Bates84", "Edlen66" or "Peck_Reeder72".

- Set King factor.
  One can use the four following settings in the "King factor" input line : "constant",

"weighted", "effective", "from file":

- "constant" - the King factor is independent of the wavelength and its value should be defined by user in the "Rayleigh depolarisation value" input line;
- "weighted", "effective" - the weighted or effective King factor will be used, respectively;
- "from file" - the wavelength dependent King factor should be given in a separate file. The path to the file containing wavelength dependent depolarisation ratio and the file name must be specified in the "Rayleigh depolarisation filename" input line.
  The file has to be consist of the header and three columns. All header lines have to be begin from ";". The first column contains the wavelength [nm] in ascending order and the second and third one the King factor and depolarization ratio, respectively.

3.14 Aerosols

Appropriate control files: "control_aer.inp", "low_aer.inp", "scia_aer.inp", "wmo_aer.inp", "man_aer.inp", "mie_aer.inp", "mod_aer.inp"
Relevant control parameters: "Aerosol settings", "Additional aerosol OT", "Add level at boudary layer top" "Aerosol OT at reference wavelength", "Aerosol parameterization type", "Aerosol scaling parameter", "Aerosol scaling factor", "Aerosol scattering matrix output", "Extinction coefficient wavelength interpolation technique", "Output of aerosol OT", "Path to aerosol data base", "Path to the tropopause height database", "Replace aerosol extinction", "Top of aerosol layers", "Use Henyey-Greenstein parameterization of scattering function?", "Use ECSTRA model"

Scattering and absorption by aerosols is considered in the radiative transfer calculations if "Aerosol settings" flag is set to "advanced" or "default" in the main control file "control.inp". If "Aerosol settings" flag is set to "off" aerosol will be switched off.

If "Aerosol settings" flag is set to "default" then default aerosol setup will be used automatically by the program (no action from user is needed). Corresponding settings can be found in Sections 3.14.2 and 3.14.4 in the scalar and vector case, respectively.

If "Aerosol settings" flag is set to "advanced" the user should define at first the general aerosol parameters in the file "control_aer.inp".

3.14.1 General settings

Appropriate control files: "control_aer.inp"

There are following options:

- Use aerosol optical parameters from database or define manually.
  Setting in the "Aerosol parameterization type" input line "lt", "st", "wm", "mi", "mod-l", "mod-o", "mod-m", or "mn"
  LOWTRAN (Shettle and Fenn, 1979; Kneizys et al., 1986), SCIATRAN (Hoogen, 1995;

Kauss, 1998), WMO (**?**), based on the incorporated Mie code, MODIS aerosol parameterization over land ("mod-l") and over ocean ("mod-o"), MERIS aerosol parameterization based on the maritime aerosol network, or the user-defined aerosol parameterization, respectively, is selected. The LOWTRAN, SCIATRAN, and WMO aerosol parameterization requires additionally the path to the aerosol database which should be specified in the "Path to aerosol data base" input line. The Mie parameterization is based on the application of Mie-code for the calculation of scattering properties of spherical particles and, therefore, is time consuming.

Limitations:

- LOWTRAN and SCIATRAN parameterizations can be used in the scalar case only;
- LOWTRAN parameterization enables the Henyey-Greenstein phase function to be used only;
- the maximal number of the phase function moments stored in SCIATRAN aerosol database is limited to 50.

- Should be aerosol layers counted from the see surface?.
  User can select from which level aerosol layers altitudes should be counted. If "Top of aerosol layers" input parameter is set to "from sea level" or to "from local surface" then top of aerosol layers will be counted from the sea level or from a local surface height, respectively.
  Attention:
  - If "Top of aerosol layers" input parameter is set to "from local surface" then:
    - the bottom of the aerosol boundary layer corresponds to the local surface height;
    - top altitudes of all aerosol layers will be shifted automatically up by the value of local surface height;
    - if the position of shifted aerosol layers does not match levels of the main altitude grid (see Section 3.3) then the top of aerosol layer will be set by the program to the nearest main altitude grid. SCIATRAN produces the warning-message

      ```
      *** WARNING in GT_CHECK:
          The top altitude of aerosol layer    2
          does not match exactly the required value
          required :  31.63 km
          used     :  30.00 km
      ```

    In this example 31.63 km and 30.00 km denote the top of the shifted second aerosol layer and the height of nearest main altitude grid, respectively, i.e., the top altitude of second aerosol layer is set by the program to 30 km.
  - If "Top of aerosol layers" input parameter is set to "from sea level" but "Height above sea level" parameter in the "control.inp" file is set to a value z_{el} large than 0 km then:
    - The aerosol below z_{el} will be cut off. Thus, e.g., if z_{el} corresponds to the top of the aerosol boundary layer, this aerosol layer will be completely omitted.
    - The aerosol layers top altitudes greater than z_{el} will not be changed.

- Use exact value for the top of boundary aerosol layer.
  Setting the "Add level at boudary layer top" control parameter to "t", user forces the program to perform radiative transfer calculation for the exact value of the boundary aerosol layer top altitude.

Attention:

- This option leads to the modification of the main altitude grid (see Section 3.3).

- Select the aerosol scattering function.
  The Henyey-Greenstein phase function can be selected in the scalar case if one set "yes" in the "Use Henyey-Greenstein parameterization of scattering function?" input line. Otherwise, the Mie phase function will be used.
  Limitations:
  - this setting has no effect if the user-defined aerosol parameterization is selected ("Aerosol parameterization type" control parameter is set to "mn").

- Wavelength interpolation of aerosol optical parameters.
  The aerosol optical parameters such as extinction coefficient, single scattering albedo, and scattering function are given usually at a discrete wavelength grid. Interpolation on a desired wavelength of single scattering albedo and scattering function is performed using linear interpolation technique. The interpolation of extinction coefficient can be performed using the linear interpolation technique also or alternatively the local Angstrom parameterization. In the forme case the extinction coefficient at wavelength $\lambda \in [\lambda_i, \lambda_{i+1}]$ is calculated according to

$$\sigma(\lambda) \;=\; \sigma(\lambda_i) \left(\frac{\lambda_i}{\lambda}\right)^p \;, \tag{3.1}$$

  where parameter p is defined as

$$p \;=\; \frac{\ln \sigma(\lambda_i)/\sigma(\lambda_{i+1})}{\ln \lambda_{i+1}/\lambda_i} \;, \tag{3.2}$$

  and $\sigma(\lambda_i)$ and $\sigma(\lambda_{i+1})$ are extinction coefficients at the wavelength λ_i and λ_{i+1}, respectively.
  User can switch between these two options setting in the "Extinction coefficient wavelength interpolation technique" input line "Linear" or "Angstrom", respectively.

- Scaling aerosol scattering and absorption coefficients.
  The specified aerosol loading can be changed scaling the aerosol scattering and absorption coefficients. The scaling factor determined by the "Aerosol scaling parameter" input line is the same for all wavelengths. The aerosol scattering and absorption coefficients will be *multiplied* by this factor at all altitudes level and all wavelengths.

- Scaling aerosol scattering and absorption coefficients in a given altitude range.
  The specified aerosol loading and the single scattering albedo can be changed scaling the aerosol scattering and absorption coefficients in any desired altitude range. This option can be used if the first entry of "Aerosol scaling factor" input line is set to "t" (true). The scaling factor determined by the second entry of "Aerosol scaling factor" input line is the same for all wavelengths and will be applied by the program in the amplitude range defined by the fourth and fifth entry parameters.
  The third entry parameter allows to change the photon absorption probability:

$$\beta \;=\; f\,\bar{\beta}\,, \tag{3.3}$$

where $\bar{\beta}$ and β are the specified and scaled photon absorption probability, f is the third entry of "Aerosol scaling factor" input line. We remind the reader that the photon absorption probability and the single scattering albedo, ω, is related as follows:

$$\beta \;=\; 1-\omega\,. \tag{3.4}$$

The perturbed ω can be also found. Substituting Eq. (3.4) into Eq. (3.3), we have

$$\omega \;=\; 1-f\,(1-\bar{\omega})\,. \tag{3.5}$$

Limitations:

- The perturbation of the single scattering albedo can be performed in the altitude range where $\bar{\omega} \neq 1$.

- Scaling aerosol particle number density.
This scaling option is relevant only if "Aerosol parameterization type" is set to "mi".
If first entry of the "Use reference extinction coefficient profile" is set to "t" (true) the next two entries will be used by program as the reference wavelength in [nm] (λ_r) and filename, which contain aerosol extinction coefficient at this wavelength within selected altitude range, $k_e(z,\lambda_r)$. The aerosol particle number density will be calculated by the program as $N(z) = k_e(z,\lambda_r)/\sigma_e(z,\lambda_r)$, where $\sigma_e(z,\lambda_r)$ is the aerosol extinction cross-section calculated by the program according to selected aerosol type (see Sect. 3.14.6).

- Setting the aerosol optical thickness manually.
User can define the desired aerosol optical thickness at a given reference wavelength. If the first value in "Aerosol OT at reference wavelength" input line is set to "t" (true) the next two entries will be used by program as the required aerosol OT and the reference wavelength in [nm].
User can define a number of additional aerosol OT for which the program calculate reflected or transmitted intensities of radiation field. If the first integer value N in "Additional aerosol OT" control line is larger than 0 then N following entries will be considered by the program as additional aerosol OT. The program calculates intensity for N+1 aerosol OT simultaneously. This option will be ignored if:
- the first entry in "Additional aerosol OT" is set to 0;
- the first entry in "Aerosol OT at reference wavelength" is set to "f" (false).
This option can be helpful performing e.g. the calculation of lookup-table.

- Replace aerosol scattering and extinction coefficients in stratosphere.
User can replace standard setting of aerosol scattering and extinction coefficients in stratosphere by specific volcanism dependent ECSTRA model profiles as given by (Fussen and Bingen, 1999). If the first value in "Use ECSTRA model" input line set to "t", the second control parameter must specify the mean optical depth of the atmosphere which will be used to calculate the volcanism parameter. The model has the best performance between 300 and 1020 nm. If this model is used the path to the tropopause height database should be defined in the "Path to the tropopause height database" input line.
Limitations:
  - below 300 nm and between 1020 and 1100 nm a spectral interpolation is performed;
  - the ECSTRA model must not be used at wavelenghts longer than 1100 nm.

- User-defined aerosol scattering coefficient profile.
  By setting the first entry in the "Replace aerosol extinction" control line to "t" the vertical profile of the aerosol extinction coefficient is replaced by values read from the file whose name is defined by the second entry. Aerosol absorption coefficient is set to zero. All other aerosol parameters are kept unchanged (i.e. set according to the parameterization selected above). File format:
  - first line: number of wavelengths;
  - second line: wavelength grid [nm];
  - subsequent lines: line number in the first column, altitude [km] in the second column and scattering coefficients [km^{-1}] for all wavelengths in other columns.

- Output of aerosol scattering matrix.
  The scattering function/matrix as function of scattering angle can be written in an output file if in "Aerosol scattering matrix output" input line one set "t". The input field is shown in the following example:
  ```
  Aerosol scattering matrix output
  t
  1  12  90   'E'
  '.DATA_OUT/Phase_matr.out'/
  ```
  where the second line after "Aerosol scattering matrix output" contains four entries: aerosol layer number, aerosol wavelength grid number, number of scattering angles, and equidistant ('E') or Gauss ('G') grid should be used for representation of scattering matrix. In the third input line the path and output-file name should be defined.

- Output of aerosol optical thicknesses at selected wavelengths.
  The aerosol optical thicknesses can be written in the output file "./DATA_OUT/AEROSOL_OUT" at user-defined discrete wavelengths. The number of wavelengths which will be used is defined as first entry in the input line "Output of aerosol OT". Other entries in this line define wavelengths in [nm]. The following example:
  ```
  Output of aerosol OT
  2  480. 550.
  ```
  shows that aerosol optical thickness will be put in the file "./DATA_OUT/AEROSOL_OUT" at the wavelengths 480 and 550 nm.

3.14.2 LOWTRAN aerosol parameterization

Appropriate control files: "low_aer.inp"

If "lt" is set in "Aerosol parameterization type" input line in the file "control_aer.inp" the LOWTRAN aerosol parameterization will be used. The parameters of desired aerosol type should be defined in the control file "low_aer.inp". They are listed in Table 3.2. Default aerosol settings ("Aerosol settings" flag is set to "default") in the case of the scalar RT computations are shown by green color in this table.
Limitations:

- LOWTRAN aerosol database is given at 18 reference wavelengths in the spectral range 200 nm - 6 μm. The wavelength grid is given in the file "DB_LT_WL.dat" located in the directory "/DATA_BASES/AEROSOLS/LT/";

Table 3.2: LOWTRAN aerosol parameterization setup (control file "low_aer.inp"). Default setting is marked by the green color.

Input line	Possible value	Meaning
Season	1, 2	Fall/Winter, Spring/Summer
Boundary layer 0 - 2 [km]		
Boundary layer aerosol type	1, 2, 3, 4	rural, urban, maritime, tropspheric
Boundary layer visibility	1, 2, 3, 4, 5	50, 23, 10, 5, 2 km
Boundary layer humidity	1, 2, 3, 4	0, 70, 80, 99 [%]
Troposphere 2 - 10 [km]		
Tropospheric visibility	1, 2	50, 23 km
Tropospheric humidity	1, 2, 3, 4	0, 70, 80, 99 [%]
Stratosphere 10 - 30 [km]		
Stratospheric aerosol loading	1, 2, 3, 4	background, moderate, high, extreme volcanic
Stratospheric aerosol type	1, 2, 3	background, aged volcanic, fresh volcanic
Mesosphere 30 - 100 km		
Mesospheric aerosol loading	1, 2	normal, transition from volcanic to normal

Table 3.3: Input field of aerosol type definition (control file "scia_aer.inp")

Input field	Comment
Name of the aerosol type	e.g., 'maritime','rural' ($\leq$ 30 characters)
N_c	number of aerosol components ($\leq$ 4)
Id_1, Rc_1 $\vdots$ $\vdots$ Id_{N_c}, Rc_{N_c}	identification number, relative particle number density
	blank line

- the number and top altitudes of aerosol layers are fixed (see Table 3.2) and can be not changed by user.

Attention:

- Top altitudes of all aerosol layers will be shifted automatically up by the value of local surface height if "Top of aerosol layers" input parameter is set to "from local surface" (see Section 3.14.1).

3.14.3 SCIATRAN aerosol parameterization

Appropriate control files: "sc_aer.inp"

If "Aerosol parameterization type" in the control file "control_aer.inp" is set to "st" the aerosol parameters have to be defined by user in the file "scia_aer.inp". There are the following options:

- Aerosol layers.
  The "Aerosol layers (SCIA_AER)" control parameter first input line contains top altitudes [km] (in the ascending order) and second input line relative humidities [%] of all aerosol layers.
  Limitations:
  - The following discrete values of the relative humidities
    0, 50, 70, 80, 90, 95, 98, and 99 [%] are allowed only.
  - Bottom of the lowest aerosol layer is assumed to be on the surface.
- Select aerosol type in all layers.
  User should define for each layer (starting at the earth surface) the aerosol type. The definition consists of several input lines after "Aerosol type definition (SCIA_AER)" input line. The structure of input field for an aerosol layer is given in Table 3.3. The available aerosol components and their identification number are given in Table 3.4.
- Define vertical profile of aerosol particles.
  The vertical profile can be given in the form of extinction coefficient (expressed in [km^{-1}]) or aerosol particle number density [particles cm^{-3}]. User can switch between these two options setting in "Profile type (SCIA_AER)" input line "exti" or "part", respectively.

Table 3.4: Aerosol components identification numbers (Id) (control file "scia_aer.inp")

Identification number	Aerosol component
1	Water soluble
2	Sea salt (accumulation mode)
3	Sea salt (coarse mode)
4	Sulfate
5	Insoluble (dust)
6	Soot
7	Mineral (nucleation mode)
8	Mineral (accumulation mode)
9	Mineral (coarse mode)
10	Mineral (transported)
11	Volcanic ash (fresh volcanic)
12	Meteoric dust

If "exti" option is chosen in "Reference wavelength (SCIA_AER)" input line the reference wavelength expressed in [nm] need to be defined. The vertical profile is defined in "Aerosol profile (SCIA_AER)" input line. The input format is as follows:
- input lines consist from two columns
- in the first column should be given altitudes [km]
- in second extinction coefficients or particle number density depending on option "exti" or "part" used in "Aerosol profile (SCIA_AER)" input line.
Attention:

- The altitudes where extinction coefficient or aerosol particle number density are given will be shifted automatically up by the value of local surface height if "Top of aerosol layers" input parameter is set to "from local surface" (see Section 3.14.1).

Limitations:

- SCIATRAN aerosol database is given at 50 reference wavelengths in the spectral range 225 nm - 2.5 μm. The wavelength grid is given in the file "DB_SC_WL.dat" located in the directory "/DATA_BASES/AEROSOLS/SCIA/".

3.14.4 WMO aerosol parameterization

Appropriate control files: "wmo_aer.inp".
If "Aerosol parameterization type" in the control file "control_aer.inp" is set to "wm" the aerosol parameters have to be defined by user in the file "wmo_aer.inp". There are the following options (default settings are shown by green color):

- Number and position of aerosol layers.
The upper boundaries in [km] of all aerosol layers are given in "WMO aerosol layers" input line in the ascending order (2., 10., 30., 60.).
Limitation:
Bottom of the lowest aerosol layer is assumed to be on the surface.
- Select aerosol type in all layers.
Desired aerosol type has to be introduced in "WMO aerosol type" input line. The possible types depend on the aerosol layer.
Boundary layer 0 - 2 [km]: urban, maritime, continental.
Troposphere 2 - 10 [km]: continental.
Stratosphere 10 - 30 [km]: background, volcanic.
Mesosphere 30 - 100 [km]: background.
- Vertical profile of aerosol extinction coefficient.
The vertical profile of the extinction coefficient can be given at a reference wavelength which has to be defined in "Reference wavelength (WMO)" input line in [nm] (550). The extinction coefficient in [km^{-1}] should be given in "Profile of extinction coefficient (WMO)" input field. The input field consists of several lines. The lines contain altitudes [km] (first column) and extinction coefficients (second column). The example of this input filed is given as (will be used as default profile)

```
Profile of extinction coefficient (WMO)
 0.0    0.025
 2.0    0.025
 3.0    0.0025
```

```
12.0    0.0025
13.0    2.18e-04
20.0    2.18e-04
30.0    3.32e-05
35.0    2.45e-05
40.0    8.00e-06
45.0    4.02e-06
50.0    2.10e-06
60.0    1.60e-07
```

Attention:

- The altitudes where extinction coefficient are given will be shifted automatically up by the value of local surface height if "Top of aerosol layers" input parameter is set to "from local surface" (see Section 3.14.1).
- The default setting will be used in the case of vector RT computations if "Aerosol settings" flag is set to "default" (see Sec. 3.14.1).

Limitations:

- WMO aerosol database is given at 61 reference wavelengths in the spectral range 200 nm - 40 μm. The wavelength grid is given in the file "WMO_DB_WL_UV-TIR.dat" located in the directory "/DATA_BASES/AEROSOLS/WMO/".

3.14.5 User-defined aerosol parameterization

Appropriate control files: "man_aer.inp"

If the "Aerosol parameterization type" input parameter is set to "mn" in the control file "control_aer.inp", then the aerosol parameters have to be defined by user in the file "man_aer.inp". The user-defined aerosol parameterization enables, in contrast to other aerosol inputs, an aerosol as a cloud layer to be considered, i.e., having sharp edges at the bottom and top of selected aerosol layer. This option is active if the "Aerosol as a cloud layer?" input parameter is set to "yes" and forces the program interpret the input field after control line "Extinction coefficient" specifically (see bel;ow).
There are the following options independent of the parameter "Aerosol as a cloud layer?":

- Top altitude of aerosol layers.
  Top altitudes [km] (in the ascending order) of all aerosol layers are given in the "Layering of scattering function/matrix" input line.
  Attention:
  - only single aerosol scattering scattering function can be defined within each aerosol layer (see below).

- Select reference wavelengths.
  To take into account the spectral dependence of scattering functions/matrices, as well as scattering and extinction coefficients the aerosol optical characteristics should be defined by user for a number of reference wavelengths. There are two possibilities within this option to define reference wavelengths:
  - Setting the first entry of "Use Angstrom parameterization" control parameter to "t", user select the wavelength dependence of scattering and extinction coefficients

according to Angstrom parameterization as follows:

$$\sigma(\lambda) \;=\; \sigma(\lambda_r)\left(\frac{\lambda_r}{\lambda}\right)^p \;, \tag{3.6}$$

where λ_r and p are the second and the third entry of the "Use Angstrom parameterization" control field.
The aerosol optical parameters, i.e., scattering matrix, extinction coefficient, and single scattering albedo can be defined below at this single wavelength only.
Attention:

- The scattering function and single scattering albedo are independent of the wavelength in this case.

- Setting the first entry of "Use Angstrom parameterization" control parameter to "f", user should define the reference wavelength grid [nm] in the ascending order in the "Wavelength grid (aerosol parameters)" input line.
  Attention:
  - at least two reference wavelengths are required;
  - the output wavelength grid (see Sec. 3.9) should be within reference wavelengths where the aerosol optical characteristics are given;
  - the wavelength interpolation is performed as described in Sec. 3.14.1.

- Select input form of scattering functions/matricies.
  Using the "Aerosol scattering function representation" input line, user can switch between three possibilities to import aerosol scattering function/matrix into the SCIATRAN code:
  - "Asymmetry_factor" - the aerosol scattering function is defined by the asymmetry factor according to the Henyey-Greenstein parameterization. The asymmetry factor should be specified for each aerosol layer and each reference wavelength in "Asymmetry factor values" input line. The input field format is given by Eq. (3.8) where $P_{i,k}$ is the asymmetry factor in the aerosol layer i and reference wavelength k.
    Limitation:
    - this option is not allowed in the vector case.
  - "Expansion_coeff" - the aerosol scattering function/matrix is represented by the Legendre (or generalized spherical functions) series expansion coefficients. The filenames containing expansion coefficients should be specified for each aerosol layer and reference wavelength in the
    "File names containing expansion coefficients" input line. The path to the directory containing corresponding files should be given in the "Directory name for scattering matrices" input line. The input field format is given by Eq. (3.8) where $P_{i,k}$ is the file name containing expansion coefficients in the aerosol layer i and reference wavelength k. The file containing expansion coefficients is formatted as follows:

    ```
    Example of the file containing expansion coefficients
    Numerical accuracy = 0.10D-06
    CEXT   = 0.339753D+01; CSCA  = 0.339753D+01
    ```

```
ALBEDO = 0.10D+01;      <COS> = 0.783276D+00
  S    Alpha 1     Alpha 2     Alpha 3     Alpha 4      Beta 1      Beta 2
>
  0    1.00000     0.00000     0.00000     0.92150     0.00000     0.00000
  1    2.34983     0.00000     0.00000     2.40089     0.00000     0.00000
  2    3.45081     4.24254     4.05375     3.35832    -0.03721     0.06524
  3    3.78591     4.29171     4.32041     3.81971    -0.07871    -0.04682
  4    4.30796     4.62039     4.53204     4.26317    -0.02429     0.06566
  5    4.54277     4.74155     4.71213     4.52701    -0.05888    -0.10526
  6    4.88813     5.08245     5.05881     4.89080     0.03230     0.03871
```

In this example first 6 lines will be considered as comment lines. In fact, the number of comment lines in the file header is arbitrary. Each line containing any character except of $0, 1, \ldots, 9, E, e, D, d$ will be considered by the program as a comment line.
The number of lines in the data block corresponds to the number of moments needed for the appropriate representation of scattering function/matrix (only seven lines is shown in the example above). The subsequent data block contain the expansion coefficients in the second - seventh columns. In the scalar case only second column will be used.
Attention:

- The reading of moments (lines) in this file will be finished if
  - end-of-file is reached;
  - all moments in a line are zero;
  - the number of moments in file greater than 5000.

– "Scattering_matrix" - the aerosol scattering function is represented as a function of the scattering angle. The filenames containing scattering functions should be specified for each aerosol layer and reference wavelength in the "File names containing scattering function/matrix" input line. The path to the directory containing corresponding files should be given in "Directory name for scattering matrices" input line. The input field format is given by Eq. (3.8) where $P_{i,k}$ is the file name containing scattering matrix in the aerosol layer i and reference wavelength k. The file containing scattering function is formatted as follows:

```
#   Example of the file containing scattering function
#   The concentration-specific volume scattering function for
#   small particles fraction corresponding to the Kopelevich model.
>
    0.0   5.3d-00
    2.0   5.1d-00
    4.0   4.6d-00
    6.0   3.9d-00
   10.0   2.5d-00
   30.0   0.2d-00
   60.0   4.1d-02
   90.0   1.2d-02
  120.0   7.4d-03
```

```
150.0   7.5d-03
180.0   8.1d-03
```

In this example first 4 lines will be considered as comment lines. The number of comment lines in the file header is arbitrary. Each line containing any character except of $0, 1, \ldots, 9, E, e, D, d$ will be considered as a comment line. The number of lines in the data block corresponds to the number of scattering angles. The first column contains the scattering angle expressed in [deg]. The second column contains the scattering function. The reading of this file will be finished if end-of-file is reached.

Attention:

- The dimension and normalization of the scattering function presented in the input file is irrelevant because the scattering matrix will be renormalized by the program as follows:

$$\frac{1}{2}\int_0^{\pi} f(\gamma)\,\sin\gamma\,d\gamma \;=\; 1\,, \tag{3.7}$$

  where $f(\gamma)$ and γ are the scattering function and scattering angle, respectively.

Limitation:

- this option is not implemented in the vector case.

Input field format for these three input option in the control file "man_aer.inp" is given by

$$\begin{array}{cccc} P_{1,1} & P_{1,2} & \ldots & P_{1,N_\lambda} \\ P_{2,1} & P_{2,2} & \ldots & P_{2,N_\lambda} \\ \ldots & \ldots & \ldots & \ldots \\ P_{L,1} & P_{L,2} & \ldots & P_{L,N_\lambda} \end{array} \tag{3.8}$$

where L is the number of aerosol layers and N_λ is the number of reference wavelengths.

- Import of extinction coefficient vertical profiles.
  In contrast to the scattering function the extinction coefficient can be defined as a function of altitude even if only single aerosol layer is selected. There is two options to input the aerosol extinction coefficient vertical profiles:
  Setting the "Source for aerosol extinction coefficients" input line to the filename containing altitude grid and extinction coefficient in [km^{-1}] (one file per wavelength).
  Setting the "Source for aerosol extinction coefficients" to the "list" for reading the aerosol extinction coefficients from the "Extinction coefficient" input field in the "man_aer.inp" file. In this case the input fields in "Extinction coefficient" input lines should be used to introduce these vertical profiles. Input field format for this option is given by

$$\begin{array}{ccccc} Z_1 & P_{1,1} & P_{1,2} & \ldots & P_{1,N_\lambda} \\ Z_2 & P_{2,1} & P_{2,2} & \ldots & P_{2,N_\lambda} \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ Z_{N_z} & P_{N_z,1} & P_{N_z,2} & \ldots & P_{N_z,N_\lambda} \end{array}$$

where $P_{j,k}$ is extinction coefficient (expressed in [km^{-1}]) at the altitude Z_j and k-th reference wavelength, Z_j is the altitude [km], N_z and N_λ is the number of altitudes and reference wavelengths, respectively.

- Import of single scattering albedo vertical profiles.
  The single scattering albedo (SSA) can be defined as a function of altitude even if only single aerosol layer is selected. The input fields in "Single scattering albedo" input lines should be used to introduce these vertical profiles. Input field format for this option is given by Eq. 3.9, where $P_{j,k}$ is SSA at the altitude Z_j and k-th wavelength. N_z is the number of altitfudes, Z_j is the altitude [km], and N_λ is the numboer of reference wavelengths.
  Attention:
  - minimum two altitude levels are required, i.e., $N_z \geq 2$;
  - the altitudes where extinction coefficient and SSA are given will be shifted automatically up by the value of local surface height if "Top of aerosol layers" input parameter is set to "from local surface" (see Section 3.14.1);
  - the aerosol extinction coefficient will be set to zero at all levels of the main altitude grid above maximal top altitude of aerosol layers.

- "Aerosol as a cloud layer?" is set to "no".
  The vertical profiles of extinction coefficients and SSA will be linearly interpolated on the altitude levels of the main altitude grid (see Section 3.3) and extrapolated with zero above the highest and below the lowest input level.
  This option does not change the main altitude grid.

- "Aerosol as a cloud layer?" is set to "yes".
  The minimal and maximal altitudes where extinction coefficient is not zero will be considered by the program as the bottom and top of the aerosol layer, respectively. The "infinitesimal" transition sub-layer above and below the aerosol layer will be incorporated by the program. Finally, the altitude grid within aerosol layer will be used instead of main altitude grid.
  In order to better explain this option let us consider the following example. The input field of the "Extinction coefficient" input parameter is given by (two reference wavelengths is assumed)

```
 Extinction coefficient
0.2     0.   0.
2.0     2.5  2.5
2.2     2.5  2.5
2.4     2.5  2.5
2.6     2.5  2.5
2.8     2.5  2.5
3.0     2.5  2.5
3.1     0.   0.
```

  The altitudes 2.0 and 3.0 km will be selected as the aerosol layer bottom and top, respectively. After introducing by the program transition sub-layers the altitude grid for aerosol layer is given by

```
1.99990      0.    0.
```

```
2.0         2.5  2.5
2.2         2.5  2.5
2.4         2.5  2.5
2.6         2.5  2.5
2.8         2.5  2.5
3.0         2.5  2.5
3.00010     0.   0.
```

i.e., the transition sab-layers of $1{\cdot}10^{-4}$ km are introduced.
All levels of the main altitude grid within interval $[1.9999 - 3.0001]$ km will be replaced by this altitude grid for aerosol layer. Thus, for instance, the equidistant main altitude grid $\{0, 2, 4, 6, \ldots, 60\}$ km will be replaced with
$\{0, 1.9999, 2.0, 2.2, 2.4, 2.6, 2.8, 3.0, 3.0001, 4, 6, \ldots, 60\}$ km grid.
This option leads to modification of the main altitude grid.
Limitation:

- The weighting functions for the aerosol layer top and bottom height cannot be calculated within this option. To do this use the option "Cloud as aerosol layer" (see Sec. 3.15.6).

Attention:

- This option is not recommended to use if the comparison of aerosol loaded and aerosol-free atmosphere should be performed because the variation of radiation field is caused not only by the impact of aerosol but also by the change of the main altitude grid.

3.14.6 Mie aerosol parameterization

Appropriate control files: "mie_aer.inp"

If "Aerosol parameterization type" in the control file "control_aer.inp" is set to "mi" the aerosol parameters have to be defined by user in the file "mie_aer.inp". This option uses the Mie code implemented into the SCIATRAN software.

Note that the original Lorenz-Mie computer program was developed by Michael Mishchenko of the NASA Goddard Institute for Space Studies, New York, and is available on-line at ftp://ftp.giss.nasa.gov/pub/crmim/spher.f. The program is described in the book Mishchenko, M. I., L. D. Travis, and A. A. Lacis (2002). "Scattering, Absorption, and Emission of Light by Small Particles", Cambridge University Press, Cambridge, which is publicly available in the PDF format at the following web site: http://www.giss.nasa.gov/ crmim/books.html.
The original version was modified by V. Rozanov to be compatible with the SCIATRAN structure and to allow for to calculate derivatives of aerosol optical parameters with respect to the parameters of lognormal particle size distribution function.

3.14.6.1 Mie parameterization in all aerosol layers

The user should define the microphysical aerosol parameters. The needed optical parameters will be calculated by SCIATRAN using the incorporated Mie code. There are following options:

- Mie aerosol layers.
  The bottom and top altitudes [km] (in the ascending order) of aerosol layers are given in the first line of "Mie aerosol layers" input field. Second input line contains relative humidities in [%] of all aerosol layers.
  Attention:
  - first value in the first input line is the bottom altitude of first aerosol layer;
  - in contrast to other aerosol parameterizations the bottom of first aerosol layer can not coincide with the surface elevation;
  - the bottom of a subsequent aerosol layer is the top of previous layer:

    ```
    Mie aerosol layers
     1.  12.  20.
       70.  50.
    ```

    This input parameters introduce two aerosol layers [1 - 12] km and [12 - 20] km with relative humidities 70% and 50%, respectively.

  Limitation: The following discrete values of the relative humidities 0, 50, 70, 80, 90, 95, 98, and 99 [%] are allowed only.

- Select desired aerosol type.
  The user should define the aerosol type within each aerosol layer. For each layer (starting at the lowest) the aerosol type definition should be done in the "Aerosol type definition (Mie)" input line. The input field consist of several lines:
  - first line contains the name of the aerosol type (string of maximal 30 characters, the program does not use this information);
  - second line contains the number N_c of aerosol components which should be listed below for a selected aerosol type;
  - the subsequent N_c lines have the following structure:

    $$\begin{array}{cccc} S_1 & D_1 & r_1 & \sigma_1 \\ S_2 & D_2 & r_2 & \sigma_2 \\ \ldots\ldots\ldots\ldots\ldots & & & \\ S_{N_c} & D_{N_c} & r_{N_c} & \sigma_{N_c} \end{array}$$

    where S_i, D_i, r_i, and σ_i are the short name, relative density, median radius [μm], and parameter of distribution width of i-th aerosol component. It is assumed that the particle size distribution function is the lognormal distribution given by

    $$\frac{dN}{dr} = \sum_{i=1}^{N_c} \frac{D_i}{r\sqrt{2\pi}\ln\sigma_i} \exp\left[-\frac{\ln^2(r/r_i)}{2\ln^2\sigma_i}\right], \tag{3.9}$$

  Attention:
  - for each layer the sum of the relative particle number densities must equal to 1;
  - the following aerosol layer must be separated by ONE e.g.
    ********** next layer **********
    dividing line.
  - The input value of the parameter r_i will be interpreted by the program depending on the "Mode radius for particle size distribution" control parameter.

- If this parameter is set to log then r_i should be considered as median radius for dN/dr;
- If this parameter is set to non-log then r_i should be considered as mode radius for dN/dr,

The maximal number of aerosol components is 14 in the current version. Their definition is given following the OPAC package in the table below (see also "mie_aer_general.inp" file). The short name, S_i, is the four first characters of names in the first column of the following table:

```
#^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
#                     Short names of aerosol components
#                    presented in the existing database
#^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
#                                                PAC recommendation -
#                                               mod. radius |  width
#                                                 micron    |  sigma
Number of aerosol components and short names
 inso-1   : insoluble                              0.471    |   2.51
 medu-1   : meteoritic dust                        0.03     |   3.16
 minm-1   : mineral (nuc.)                         0.07     |   1.95
 minn-1   : mineral (nuc.) <prolate spheroids>     0.07     |   1.95
 miam-1   : mineral (acc.)                         0.39     |   2.00
 mian-1   : mineral (acc.) <prolate spheroids>     0.39     |   2.00
 micm-1   : mineral (coa.)                         1.90     |   2.15
 micn-1   : mineral (coa.) <prolate spheroids>     1.90     |   2.15
 mitr-1   : mineral (tra.)                         0.50     |   2.20
 soot-1   : soot                                   0.0118   |   2.00
 suso-8   : sulfate          [8 humidities]        0.0695   |   2.03
 ssam-8   : sea salt (acc.) [8 humidities]         0.209    |   2.03
 sscm-8   : sea salt (coa.) [8 humidities]         1.75     |   2.03
 waso-8   : water soluble    [8 humidities]        0.0212   |   2.24
#*************************************************************************
```

Attention:

- The usage of aerosol components marked by `<prolate spheroids>` does not require Mie calculations because in contrast to the other aerosol components the data base consists of pre-calculated optical parameters such as extinction, scattering coefficients, and scattering functions at selected number of wavelengths.

- Wavelength grid to perform Mie calculations.
To perform Mie calculations the program needs a wavelength grid. The wavelength grid expressed in [nm] in the ascending order should be defined in the "Wavelength grid for the Mie aerosol parameterization" input line.
Attention:
  - at least two wavelengths are required;
  - the output wavelength grid (see Sec. 3.9) should be within wavelength grid defined for Mie calculations;

- aerosol optical parameters calculated on the wavelength grid defined for Mie calculations will be interpolated by the program on the output wavelength grid.

- Numerical integration of monodisperse optical aerosol characteristics.
  The trade-off between the speed and accuracy of the polydisperse optical aerosol parameters computation can be obtained by properly definition the lower and upper integration limits. The minimal and maximal values of the radius in [μm], where the numerical integration will be performed by the Mie code, should be defined in the "Numerical integration limits" input line. The input field consists of two entries: first entry defines the minimal and second entry the maximal radius of the integration range.

- Explicit definition of bimodal log-normal distribution.
  For the solution of some inverse problems the derivatives of the aerosol optical parameters with respect to the parameters of log-normal distribution of the fine and coarse mode are required. To calculate derivatives for both mode one needs to use the "Use bimodal" input line. If the input value is set to "t", the program calculates derivatives with respect to the median radius and width parameter of the fine and course mode separately (see Section 3.1.6).
  The "Upper boundary for fine mode" input line allows to define the maximal modal radius , R_{max}, in [μm] of the fine mode such that all aerosol components with $r_{mod} \leq R_{max}$ will be considered as the fine mode and $r_{mod} > R_{max}$ will be considered as course mode.

- Aerosol particles number density profile.
  The aerosol particle number density profile should be defined in the "Profile" input field. The input field consists of several lines:
  - each line consists of two columns: first column contains the height in [km] and second column the aerosol number density expressed in [cm^{-3}].

  Attention: The extrapolation above the highest and below the lowest input level will be performed with the zero value.

3.14.6.2 Mie parameterization in selected aerosol layers

The user can select the Mie parameterization mode to define aerosol properties in a single selected aerosol layer only, e.g., in the stratosphere. The aerosol properties outside of the selected Mie aerosol layer can be defined using another standard aerosol parameterization.
Setting in the "Aerosol parameterization type" input line "lt_mi", "st_mi", or "wm_mi", the aerosol properties outside of the selected Mie aerosol layer will be used according to LOWTRAN, SCIATRAN, or WMO aerosol parameterization, respectively.
Attention:

- The aerosol parameters according to the selected standard parameterization should be introduced as described before. The aerosol optical parameters will be overwritten within a layer (or layers) where the Mie parameterization is selected.

3.14.7 MODIS aerosol parameterization over land

Appropriate control files: "mod_aer.inp"

If "Aerosol parameterization type" in the control file "control_aer.inp" is set to "mod-l" the aerosol parameters have to be defined by user in the file "mod_aer.inp". This option uses the implemented into SCIATRAN Mie code to calculate aerosol optical parameters. However, in contrast to the Mie parameterization discussed in Sec. 3.14.6, the MODIS parameterization is based on the statistical analysis of the land global AERONET data (see (Levy et al., 2007) for details) and, therefore, enables a single aerosol layer (boundary layer) to be defined only. Moreover, in contrast to the Mie parameterization the user should define the aerosol optical thickness at 550 nm and aerosol type only.

There are following options:

- Bottom and top of aerosol layers.
  The bottom and top altitudes [km] of an aerosol layer are given in the "Bottom and top of aerosol layer (MODIS)" input line. The input field consists of two entries: first entry defines the bottom and second entry the top altitude of aerosol layer.

- Wavelength grid to perform Mie calculations.
  To perform Mie calculations the program needs a wavelength grid. The wavelength grid expressed in [nm] in the ascending order should be defined in the "Wavelength grid (MODIS)" input line.

- Select desired aerosol type.
  The user should define the aerosol type within selected aerosol layer. The input field of parameter "Aerosol type definition (MODIS)" consists of four entries:
  - first entry - fine mode aerosol type. Possible choice is "Strongly_absorbing", "Moderately_absorbing", and "Weakly_absorbing";
  - second entry - course mode aerosol type. Possible choice is "Spheroidal_(dust)";
  - third entry - aerosol optical thickness at 550 nm;
  - fourth entry - coarse mode fraction.

- Numerical integration of monodisperse optical aerosol characteristics.
  The minimal and maximal values of the particle radius in [μm], where the numerical integration will be performed by the Mie code, should be defined in the "Numerical integration limits (MODIS)" input line. The input field consists of two entries: first entry defines the minimal and second entry the maximal radius in [μm] of the integration range.

- Aerosol particles number density profile.
  The aerosol particle number density profile should be defined in the "Aerosol particle number density (MODIS)" input field. The input field consists of several lines:
  - each line consists of two columns: first column contains the height in [km] and second column the aerosol number density profile.

  Note that only shape of aerosol number density profile will be used by the program because the optical thickness of the aerosol layer is given at 550 nm.

3.14.8 MODIS aerosol parameterization over ocean

Appropriate control files: "mod_aer_oc.inp"

If "Aerosol parameterization type" in the control file "control_aer.inp" is set to "mod-o" the aerosol parameters have to be defined by user in the file "mod_aer_oc.inp". This option uses the implemented into SCIATRAN Mie code to calculate aerosol optical parameters. This parameterization is based on the statistical analysis of the MODIS data over oceans (see (Tanre et al., 1997) for details) and, therefore, enables a single aerosol layer (boundary layer) to be defined only.

There are following options:

- Bottom and top of aerosol layers.
  The bottom and top altitudes [km] of an aerosol layer are given in the "Bottom and top of aerosol layer (AER_OC)" input line. The input field consists of two entries: first entry defines the bottom and second entry the top altitude of aerosol layer.

- Wavelength grid to perform Mie calculations.
  To perform Mie calculations the program needs a wavelength grid. The wavelength grid expressed in [nm] in the ascending order should be defined in the "Wavelength grid (AER_OC)" input line.

- Select desired aerosol type.
  The user should define the aerosol type within selected aerosol layer. The input field of parameter "Aerosol type definition (AER_OC)" consists of three entries:
  - first entry - fine mode aerosol type. Possible choice is "MOD_F1.dat", "MOD_F2.dat", "MOD_F3.dat", "MOD_F4.dat";
  - second entry - course mode aerosol type. Possible choice is "MOD_C1.dat", "MOD_C2.dat", "MOD_C3.dat", "MOD_C4.dat", "MOD_C5.dat";
  - third entry - coarse mode fraction.

  The files are located in the "/DATA_BASES/AEROSOLS/MODIS_OC/" directory and contain information about modal radius, variance, wavelengths, and real and imaginary part of refractive index selected aerosol mode.

- Numerical integration of monodisperse optical aerosol characteristics.
  The minimal and maximal values of the particle radius in [μm], where the numerical integration will be performed by the Mie code, should be defined in the "Numerical integration limits (AER_OC)" input line. The input field consists of two entries: first entry defines the minimal and second entry the maximal radius in [μm] of the integration range.

- Aerosol particles number density profile.
  The aerosol particle number density profile should be defined in the "Aerosol particle number density (AER_OC)" input field. The input field consists of several lines:
  - each line consists of two columns:
    - first column contains the height in [km]
    - second column contains the aerosol number density profile in [cm^{-3}].

  Attention
  In contrast to the MODIS parameterization over land (see Section 3.14.7) the aerosol number density profile will be used by the program to calculate the optical thickness of the aerosol layer.

3.14.9 Ocean-aerosol parameterization based on the maritime aerosol network (MAN)

Appropriate control files: "mod_aer_man.inp"

If "Aerosol parameterization type" in the control file "control_aer.inp" is set to "mod-m" the aerosol parameters have to be defined by user in the file "mod_aer_man.inp". This option uses the implemented into SCIATRAN Mie code also. However, in contrast to the Mie parameterization discussed in Sec. 3.14.6, the MAN parameterization is based on the statistical analysis of the ocean global AERONET data and therefore allows to define a single aerosol layer (boundary layer) only.

There are following options:

- Bottom and top of aerosol layers.
  The bottom and top altitudes [km] of an aerosol layer are given in the "Bottom and top of aerosol layer (MODIS Mie)" input line.
- Wavelength grid to perform Mie calculations.
  To perform Mie calculations the program needs a wavelength grid. The wavelength grid expressed in [nm] in the ascending order should be defined in the "Wavelength grid (MODIS Mie)" input line.
- Select desired aerosol type.
  The user should define the aerosol type within selected aerosol layer. The input field of parameter "Aerosol type definition (MODIS Mie)" consists of two entries:
  - first entry - aerosol type. Possible choice is "Dust_influenced", "Pollution-1", "Pollution-2", and "Pure_Maritime"
  - second entry - aerosol optical thickness at 550 nm.
- Numerical integration of monodisperse optical aerosol characteristics.
  The minimal and maximal values of the radius in [μm], where the numerical integration will be performed by the Mie code, should be defined in the "Numerical integration limits (MODIS Mie)" input line. The input field consists of two entries: first entry defines the minimal and second entry the maximal radius in [μm] of the integration range.
- Aerosol particles number density profile.
  The aerosol particle number density profile should be defined in the "Aerosol particle number density (MODIS Mie)" input field. The input field consists of several lines:
  - each line consists of two columns: first column contains the height in [km] and second column the aerosol number density profile.

  Note that only shape of aerosol number density profile will be used by the program because the optical thickness of the aerosol layer is given at 550 nm.

3.15 Clouds

Appropriate control files: "control.inp" ,"cloud.inp"
Relevant control parameters: "Clouds present?"

All settings discussed in this section have only an effect if the parameter "Clouds present?" in the "control.inp" file is set to "t".
Limitation:

- Clouds are not supported if "RTM-CORE" is set to "CDI" (see Section 3.6).

Considering cloud parameters, we will use the following terminology:

- **g**eometrical parameters - cloud top height h_t, cloud bottom height h_b, and cloud geometrical thickness $h_t - h_b$.
- **c**loud layer - the part of the atmosphere between a cloud bottom and cloud top;
- **w**ater/ice cloud - cloud consisting of either water droplets or ice crystals;
- **m**ixed cloud - cloud consisting of a mixture of water droplets and ice crystals;
- **v**ertically homogeneous cloud - all optical parameters of the cloud are constant within a cloud layer;
- **v**ertically inhomogeneous cloud - optical parameters of the cloud are altitude dependent within a cloud layer;
- **i**ntegral parameters - parameters describing integral properties of a cloud layer, such as optical thickness (τ), liquid water path (LWP), ice water path (IWP);

3.15.1 General

Appropriate control file: "cloud.inp"
Relevant control parameters: "Altitude sub-grid within cloud layers", "Cloud layers are vertically inhomogeneous", "Cloud particle geometrical dimension",
"Cloud particle profile input file", "Cloud layer base and top", "Cloud sub-layers number",
"Delta-M or Delta-Fit ", "Delta-m truncation for cloud layers", "Expansion coefficients input file", "Filenames in database", "Form of ice crystals", "Ice crystal dimension range", "Lower and upper value of forward cone", "Number of cloud layers",
"Path to cloud data bases", "Phase function of cloud layers",
"Phase functions output" (temporary disabled), "Refractive index of water and ice", "Scattering and absorption coefficients", "Thermodynamic state",
"Type of input integral parameter",
"Use constant phase function within cloud layer",
"Use PSD for ice crystals"

There are following options to properly involve clouds in the radiative transfer process:

- Geometry of the desired cloud system.
  The "Number of cloud layers" input line defines the number of cloud layers to be considered in the radiative transfer computations. The case with the number of cloud layers greater than one corresponds to a multilayered cloud system.

  Value for the base and top altitudes should be defined (in km) for each cloud layer in "Cloud layer base and top" input field. In the case of a multilayered cloud system, cloud layers have to be arranged in an ascending order, i.e., from the bottom to the top of the atmosphere.
  Attention
  - The number of lines read by the program in "Cloud layer base and top" input field is equal to the number of cloud layers defined by user in the "Number of cloud

layers" input line, all subsequent lines will be ignored. This will be the case for all input fields containing cloud parameters which have to be defined for each cloud layer. In the following we will call these parameters as *l*ayer-specific.

The number of sub-layers within each cloud layer is controlled by "Cloud sub-layers number" input field. This number depends on the vertical inhomogeneity of a particular cloud layer and has to be ≥ 2. This is a *l*ayer-specific parameter.

The sub-grid level altitudes corresponding to the "Cloud sub-layers number" within cloud layer can be chosen as "equidistant" or "logarithmic" in "Altitude sub-grid within cloud layers" input line. This is a *l*ayer-specific parameter.
The option "logarithmic" is recommended to use in the case of very optically thick cloud layer (as e.g., snow layer).

The Geometrical Thickness of Transition Layer (GTTL) between cloud layer and cloud-free atmosphere can be define in the "Thickness of transition layer" control line. The following options can be selected:

- default - GTTL will be set to 10^{-4} [km];
- dynamic - GTTL will be set to GT$\cdot 10^{-4}$, where GT is selected geometrical thickness of cloud;
- any numerical value will be used by the program as user defined GTTL in [km].

Attention:

- In SCIATRAN versions less than 3.8 the GTTL value has been used by default eqal to 10^{-4} [km]. Keep in mind by the comparison of results obtained using different SCIATRAN versions.

- Refractive index of water and ice.
  The refractive index of water and ice should be given in separate files. Names of files containing refreactive index of water and ice should be given as two entries in the "Refractive index of water and ice" control line. The first entry contains filename for refractive index of water and second one for ice. Path to files is given in the "Path to cloud data bases" control line. The structure of both files is as follows:
  - first line contains the number of wavelength where refractive index is given;
  - other lines consist of three columns: first column - wavelength in [μm], second and third - real and imaginary part of refractive index, respectively.

- Select thermodynamic state of cloud layer.
  A data base availability and the way how the contents of the user-supplied file are interpreted by the program depend on the thermodynamic state of cloud layers, which is controlled by the "Thermodynamic state" input parameter. This parameter consists of two entries. First entry can be set to "water", "ice", or "mixed" defining water, ice, or mixed cloud, respectively. Second entry is an optional parameter which is relevant in combination with Yang database only and defines the number of ice habit forms used. This is the *l*ayer-specific parameter.

  If the first entry of "Thermodynamic state" parameter is set to "ice" or "mixed" the user needs to select an available form or database of ice crystals in the "Form of ice crystals" input field. This input field can consist of many input lines and each line from many entries.

First input line contains information about optical characteristics ice crystals database which will be used. The possible choice is:

- "Baum" - the Baum database for "AggregateSolidColumns" form of ice crystals is available in the spectral range 0.2 - 99.0 μm for effective radii in the range 5 - 60 μm;
- "Fractal" - optical characteristics of fractal particle of the second generation on the base of a regular tetrahedron were precalculated for discrete edge lengths of tetrahedron equal to 50, 100, and 300 μm in the spectral range 0.3 - 41.1 μm;
- "Hexagon" - optical characteristics of hexagonal prisms were precalculated for single height of 100 μm and discrete side lengths of 12.5, 25, 50, 200, 400, and 800 μm in the spectral range 0.3 - 41.1 μm;
- "Yang" - Yang database is available in the spectral range 0.2 - 15.25 μm for maximal dimension of ice habits in the range from 2 to 10 000 μm. Only 1000 expansion coefficients of scattering matrix elements were saved in the SCIATRAN database. Therefore, it is recommended to use in combination with this database the single-scattering correction algorithm (see Section 3.7.5);

If the first entry in the first input line is set to "Yang", then the second entry in this line need to be set to "yes", or "no" defining if the program uses or does not use the original scattering matrix in the single scattering correction algorithm (see Section 3.7.5). It is recommended to set "yes" in second entry of the "Form of ice crystals" input line.
If the first entry in the first input line of the "Form of ice crystals" parameter is set to "Baum", "Fractal" or "Hexagon", then other input lines will be ignored.

- Options specific by usage of "Yang" database.
  Selection of Yang database offers following additional options to handle optical parameters of ice crystals.
  - Form of ice crystal and crystal surface roughness.
    The second input line is used to define the discrete grid of maximal dimension where relative concentration of selected ice crystal is given. The content of this input line depends on the setting in second entry of the "Thermodynamic state" parameter. If the number of ice habit forms is set to 1, then two following settings are identical:
    1)
    ```
    --- Layer --->
    column_8elements  050  1.0  1.0
    ```
    2)
    ```
    --- Layer --->          100. 500.
    column_8elements  050  1.0  1.0
    ```
    are identical. This means that in the second input line can be given or not given the discrete grid of maximal dimension.
    In the next input line the user can select forms of ice crystals that will be used
    - first entry defines selected form of ice crystal habit; The following settings in the first entry are allowed: "column_8elementss" - aggregate of 8 columns; "droxtal" - droxtal; "hollow_column" - hollow column; "hollow_bullet_rosette" - hollow bullet rosette; "plate" - plate; "plate_10elements" - aggregate of 10 plates; "plate_5elements" - aggregate of 5 plates; "solid_column" - solid col-

umn;
"solid_bullet_rosette" - solid bullet rosette;

- second entry can be set to "000", "003", or "050" defining the crystal surface roughness as smooth, moderately roughened, and severely roughened, respectively;
- other entries define the relative concentration of selected ice crystal form in the mixture at basic grid of dimensions, We note that in the case 1) two values are required.

- Snow grain habit mixture model.
  If the number of ice habit forms (second entry of the "Thermodynamic state" parameter) is larger than 1, then the user should define a snow grain habit mixture model. In this case the second line of the input field "Form of ice crystals" has to be contain the discrete grid of maximal dimensions where relative concentration of selected ice crystal form is given.
  Let us consider the case where snow particles shape varies with the particle size.

```
--- Layer --->                100    300   1000   3000
column_8elements       050    0.9    0.2   0.0     0.0
solid_bullet_rosette   050    0.0    0.2   0.3     0.0
droxtal                050    0.1    0.6   0.7     1.0
```

  The particular size division points are given at $D = 100, 300, 1000$, and $3000\,\mu$m. Snow particle habit fractions are given at the same division points and vary linearly with respect to logarithmic maximum dimension between particular size division points and extrapolated as constant to the minimal ($2\,\mu$m) and maximal ($10000\,\mu$m) dimension of the Yang database. Thus, e.g., the droxtal fraction is selected as constant between $2\,\mu$m and $100\,\mu$m and equal 10%, increases from 10% till 100% between $100\,\mu$m and $3000\,\mu$m, and remains constant between $3000\,\mu$m and $10000\,\mu$m.
  The number and values of division points can be selected by user.
  Attention:
  - At least two division points should be defined.
  - The sum of particle habit fractions at each division points should be equal to 1.

  It is the *l*ayer-specific parameter.

- Polydisperse ice particles.
  Setting first entry of the "Use PSD for ice crystals" parameter to "f" or "t", the user can switch between monodisperse or polydisperse optical characteristics. If first entry of the "Use PSD for ice crystals" parameter is set to "t", the Gamma-distribution function will be employed to describe polydisperse structure of ice crystals:

$$n(D) \;=\; N_0 \left(\frac{D}{D_0}\right)^{k-1} \exp\left[-(k-1)\,\frac{D}{D_0}\right] \;, \tag{3.10}$$

  where k is the shape parameter, D_0 is the mode, and the normalization factor is

$$N_0 = \frac{(k-1)^k}{(k-1)!\,D_0} \;. \tag{3.11}$$

It is worth to notice that we introduced the mode D_0 instead of scale parameter v utilized in (Saito et al., 2019). The relationship between these parameters is

$$D_0 \;=\; (k-1)\,v\;. \tag{3.12}$$

The mode D_0 can be selected as constant within cloud layer or depending on the altitude (see below in "Select vertically homogeneous or inhomogeneous clouds").
If one needs to use only small range of ice crystal dimensions (as e.g., in the case of vertically homogeneous monodisperse layer), it is reasonable to use the "Ice crystal dimension range" parameter. The input field of this parameter consist of three entries.
If the first entry is set to "off", the other entries will be ignored.
If the first entry is set to "on", second and third entries define minimal (d_{min}) and maximal (d_{max}) values of dimension. The optical parameters of ice crystals will be read in this case only in the range $[d_{min}, d_{max}]$.
This option speed up the reading of optical parameters especially scattering matrices and expansion coefficients.

Limitation:

- if "Thermodynamic state" of any cloud layer is set to "ice" the "Form of ice crystals" has to be defined for each cloud layer, although it will be ignored in the cloud layers where "Thermodynamic state" is set to "water";

Attention:

- It is also possible to calculated radiative transfer through cloud consisting of aerosol particles (aerosol cloud) rather than water droplets or ice crystals. This option can be used setting the control parameter "Thermodynamic state" to "alay". The detailed description of this option is given below.

- Select vertically homogeneous or inhomogeneous clouds.
User can select vertically homogeneous or inhomogeneous clouds. This can be done setting in the first entry of "Cloud layers are vertically inhomogeneous" input line "no" or "yes", respectively. Second entry is an optional parameter.

  If the first entry of "Cloud layers are vertically inhomogeneous" parameter is set to "no", all cloud layers will be considered as vertically homogeneous. The second entry can be empty in this case or set to "file" or "const". In this case the program does not need the input information about the shape profiles of liquid water content, ice water content, and particle number density (they will be set to unit automatically). The information about the geometrical dimension of cloud particles
  - effective radius of water droplets,
  - side length and height of hexagonal prism,
  - edge length of fractal crystals,
  - effective radius of aggregated solid columns,
  - maximal dimension for ice habits from Yang database

  in each cloud layer has to be given in "Cloud particle geometrical dimension" input line as follows:

```
# ------------------------------------------------------------
#|  Water  |                      Ice                         |
```

```
# ------------------------------------------------------------
#|          |   Hexagonal prism     | Fractal (edge length) |
#| Radius   | Side length | Height  |    Baum DB (R_eff)    |
#|          |             |         |    Yang DB (Dim)      |
#------------------------------------------------------------
Cloud particle geometrical dimension
     16.           50.   100.            100.
# ------------------------------------------------------------
```

Attention

- the height of the hexagonal prism in the current version can be set to 100 μm only;
- fourth entry will be used by the program as edge length for fractal, effective radius for Baum database (aggregated solid columns), or maximal dimension for ice habits from Yang database.

The geometrical dimension of cloud particles will be used by the program to calculate liquid/ice water content or particles number density depending on the chosen value of "Type of input integral parameter" (see below).

Limitation:

- the "Type of input integral parameter" control line can only be set to "TAU" or to "WATER_PATH" in this case.

If the first entry of "Cloud layers are vertically inhomogeneous" parameter is set to "yes", all cloud layers will be considered as vertically inhomogeneous. The second entry of "Cloud layers are vertically inhomogeneous" parameter should be set to "file", "const" or may be empty.
If the second entry is set to "file" or empty than the information about the vertical profiles of the basic cloud parameters in each cloud layer has to be given in a separate file. Parameter "Cloud particle profile input file" defines the corresponding file name. In the current version this parameter can be set e.g., to "cld_prof_inp.vin".

```
*  Example of the file structure "cld_prof_inp.vin".
*  1st column - dimensionless height variable from the cloud top
*               to the cloud bottom: (z_top - z)/(z_top - z_base)
*  2nd        - shape of liquid-water content or particle concentration
*  3th        - profile of droplets radius [micron]
*  4th        - shape of ice-water content or crystal concentration
*  5th        - side length of hexagonal prism [micron]
*  6th        - height of hexagonal prism (100 micron only!!)
*  7th        - edge length of regular tetrahedron [micron] (for fractal)
*               effective radius [micron] (aggregated solid columns)
*               maximal dimension [micron] (Yang database)
*---------------------------------------
* Z |  Water |          Ice            |
*---------------------------------------
* 1   2     3     4      5     6     7
>
0.   0.355  20.  0.0575   50.  100.   50.
0.5  0.555  16.  0.0575   75.  100.   50.
```

```
1.   0.755  10.  0.0575  100.  100.   50.
```

The general structure of these file is as follows:

- all lines before the line containing symbol ">" are treated as comment lines;
- the first column contains the dimensionless altitude from the cloud top to the cloud bottom: $(z_{top} - z)/(z_{top} - z_{base})$ (at least 3 altitude levels must be defined);
- the content of the second column depends on the setting in the "Type of input integral parameter" control field for water cloud (see below);
- the third column contains the profile of the water droplet effective radius [μm];
- the content of the fourth column depends on the setting in the "Type of input integral parameter" control field for ice cloud (see below);
- the fifth column contains the profile of the side length of the hexagonal ice crystal [μm];
- the sixth column contains the height of the hexagonal prism (in the current version it can be set to 100 μm only);
- the seventh column contains (depending on the selected ice crystal form):
  - the edge length [μm] of regular tetrahedron for fractal,
  - effective radius [μm] of aggregated solid columns,
  - maximal dimension [μm] of ice habits from Yang database.

If the second entry is set to "const" than the information about the vertical profiles of the basic cloud parameters in each cloud layer will be defined by the same way as in the case of a vertically homogeneous cloud (see above).

- Select scattering function/matrix and scattering, extinction cross-sections of cloud layer.

Generally, there are two ways to select phase function and scattering, extinction cross-sections of cloud particles:

- use a pre-calculated database containing extinction cross-section, single scattering albedo, and phase function moments at a discrete wavelength grid;
- supply a user-defined file containing phase function moments, extinction and scattering cross-section. In this case cloud optical parameters independent of the wavelength.

Setting in "Phase function of cloud layers" input line "db" or "user", one can switch between this two options. This is a *l*ayer-specific parameter.

If option "db" is selected, then the program will read scattering function moments from the database appropriate to the selected type of the cloud. The filenames should be specified in "Filenames in database" input line. The appropriate filenames can be given as below:

"Thermodynamic state" is set to "water"	"Thermodynamic state" is set to "ice"'
"Greek-{effective radius}", where effective radius of water droplets can be set to: 2, 4, 6, ..., 40 μm, i.e., for example, the entry "Greek-8" will select from the data base the extinction coefficient, single scattering albedo, and phase function moments appropriate to a water cloud with an effective radius of water droplets of 8 μm.	"Greek_Fractal_X" for fractal, where X is the edge length of regular tetrahedron: 50, 100, 300 μm; "Greek_Hexagon_L100_rX" for hexagonal crystals, where X is side length of hexagonal prism: 12.5, 25, 50, 200, 400, 800 μm; "AggregateSolidColumns_EK_X" for aggregated solid columns, where X is the effective radius: 5.00, 7.50, 10.0, 12.5, ..., 60.0 μm; "{ice_crystal_habit name}_X" for Yang database, where X is maximal dimension.

For example, the entry "Greek_Hexagon_L100_r12.5" will select from the data base the extinction coefficient, single scattering albedo, and phase function moments appropriate to an ice cloud consisting of hexagonal crystals with height of hexagonal prism (L) of 100 μm and side length of 12.5 μm.

The path to the database has to be given in "Path to cloud data bases" control line. Attention:

- Note that the control line "Filenames in database" must always contain both file names, i.e., the first for water droplets and the second for ice crystals, independent of the desired cloud type.

If option "user" is selected in "Phase function of cloud layers" input line, then the program will read scattering, extinction cross-sections, and scattering function/matrix moments from the user-defined file. In order to supply user-defined optical characteristics, the name of the file containing the extinction, scattering cross-sections, and moments of the scattering function/matrix of the water and ice particles has to be specified in "Expansion coefficients input file" control line. The structure of these files is as shown in following example:

```
NUMERICAL ACCURACY = 0.10D-06
GAMMA DISTRIBUTION,  a = 10.0000  b = 0.1111
*********   EXPANSION COEFFICIENTS   *********
   S     ALPHA 1    ALPHA 2    ALPHA 3    ALPHA 4     BETA 1     BETA 2
>
      0.456293D+03   0.456292D+03
   0     1.00000    0.00000    0.00000    0.95342    0.00000    0.00000
   1     2.58533    0.00000    0.00000    2.62204    0.00000    0.00000
   2     3.95726    4.51125    4.39437    3.90539   -0.00162    0.02081
```

The input file must contain a line with ">" as the first symbol, which separates the

header from the data block. The header can contain arbitrary number of lines. The first line below this separation line must contain two values which will be interpreted as the extinction and the scattering cross-sections (should be given in $[\mu m^2]$), respectively. This line is followed by a two-column or seven-column data block in the scalar or vector case, respectively. The number of lines corresponds to the number of moments (N) needed for the appropriate representation of scattering function/matrix (only three lines are shown in the example above). The expansion coefficients of the scattering function or matrix are in 2nd or in 2-7th columns. The first column is ignored during the reading.
Attention:

- Note that the control line "Expansion coefficients input file" must always contain both file names, i.e., the first for water droplets and the second for ice crystals, independent of the desired cloud type.
- The reading of moments (lines) in the user-defined file will be finished when
  - end-of-file has been reached;
  - the number of read moments is greater than 10000.
- It is assumed that the expansion coefficients contain common multiplier $2k + 1$, where $k = 0, 1, \ldots, N$

Setting "Phase function of cloud layers" to "hg" or "iso", the cloud phase function will be converted to a phase function of Henyey-Greenstein type deriving the appropriate asymmetry parameter from the second Legendre moment contained in the selected cloud database (as defined in "Filenames in database" input line) or to an isotropic phase function, respectively.

- Dependence of the scattering function on effective radius of cloud particles.
  The scattering function can be used as a constant or variable within a cloud layer. Setting the parameter "Use constant phase function within cloud layer" to "t" or to "f" one switches of or on the dependence of the phase function on the effective radius.
  Limitations:
  - this option is available
    - for water clouds if the parameter "Phase function of cloud layers" is set to "db",
    - for ice cloud if the first entry of the first line "Form of ice crystals" parameter is set to "Baum" or to "Yang";
  - the phase function of an ice cloud consisting of fractal particles or hexagonal prisms and mixed clouds has to be constant within a cloud layer but can be different for different cloud layers;
  - this option can not be used if the paramete "RTM_TYPE" is set to "spher_scat";
  - Delta-M truncation technique is allowed only (see below) if parameter "Use constant phase function within cloud layer" is set to "f".

- Select truncation technique of scattering function.
  Changing the setting of "Delta-M or Delta-Fit" control parameter between "D-M" and "D-F" user can switch between Delta-M approximation (Wiscombe, 1977) and Delta-Fit approach (Hu et al., 2000), respectively. This setting is valid for all cloud layers. Only one input line is required.

  If "D-M" option is chosen, then a desired number of scattering function moments, which will be used to approximate the full scattering function within a cloud layer, is controlled

by "Delta-m truncation for cloud layers" parameter. This is a *l*ayer-specific parameter. Attention:

- If required value of the "Delta-m truncation for cloud layers" parameter is larger than the default value 34, the user needs:
  1) set the "Advanced accuracy control" parameter to "t" ("control.inp" file);
  2) set in the "Number of Legendre moments" input line ("control_ac.inp" file) the value greater than at least "Delta-m truncation for cloud layers" + 1;
  3) set in the "Number of streams" input line corresponding value of streams (see Section 3.7.4).

If "D-F" option is chosen, then the dimension of the forward cone used for truncation of the scattering function has to be defined. The first and second entry in the "Lower and upper value of forward cone" input line contain the range values of the desired forward cone in [deg]. If the difference between upper and lower values is larger than 0.1°, the quasi-optimal value of the forward cone will be found automatically by the program. If this difference is smaller than 0.1° the first entry in ' 'Lower and upper value of forward cone" input line will be used as the forward cone dimension.

Limitations: The Delta-Fit approach ("D-F") is available in the scalar case only.

- Define scattering and extinction coefficients.
  There are three options to calculate scattering and extinction coefficients within cloud layers, i.e., employing analytical formulae, using scattering and extinction cross-section from corresponding database or from an user-defined input file.
  By choosing either "analytically" or "from data base" in the control line "Scattering and absorption coefficients" the user can switch between analytical calculation and usage of database or user-defined cross-sections.

  Limitations: If weighting functions for such cloud parameters as ice water content, crystal number density, and effective radius should be calculated, only option "analytically" is allowed if form of ice crystal is set to "Fractal" or "Hexagon".

  If option "analytically" is chosen, the calculation of the scattering and extinction coefficients requires liquid/ice water content LWC(z)/IWC(z) and effective radius profiles within a cloud and will be performed employing simple analytical approximate formulas as given in (Kokhanovsky, 2004a).

  If option "from data base" is chosen, the calculation of scattering and extinction coefficients requires particle number density profile N(z) and cross-sections from database or from an user-defined input file. The corresponding scattering and extinction coefficient will be obtained as product of cross-section and particle number density profile N(z).

  The approach used to calculate LWC(z)/IWC(z) and N(z) within a cloud layer depends on the setting of control parameter "Type of input integral parameter".
  For a water or ice cloud "Type of input integral parameter" can be set as follows:
  - "TAU" - optical thickness at the reference wavelength 500 nm;
  - "WATER_PATH" - liquid/ice water path [g m^{-2}];
  - "LWC_PROFILE"/"IWC_PROFILE" - liquid/ice water content profile [g m^{-3}];
  - "DENS_PROFILE"- particles/crystals number density profile [cm^{-3}].

The input line consists of two entries. The first entry defines the input integral parameter for water clouds and second one for ice clouds. The approach to calculate LWC(z)/IWC(z) and N(z) is described below in details.

3.15.2 Water clouds: "Type of input integral parameter"

Appropriate control file: "cloud.inp"
Relevant control parameters: "Input integral parameter", "Will be scaled vertical profile of"

"TAU"
A cloud layer is characterized by its optical thickness, τ, at the wavelength 500 nm. Although the optical thickness is defined by the first input value ("TAU" field) in the "Input integral parameter" control line, three additional input entries must be given in the same control line, even though they will not be used in the calculations (see example below).

```
## ------------------------------------
## |                                   |
## |----  Water ------|------  Ice -----|
## |  TAU   |    LWP  |    TAU  |   IWP |
##
Input integral parameter
     20.0      42.477     1.0     8.431
## ------------------------------------
```

The required cloud optical thickness can be obtained scaling the shape of LWC or particle number density N(z) profiles. The user can switch between these two possibilities setting in control line "Will be scaled vertical profile of" either "Scale-WC" or "Scale-NC". Setting "Scale-WC" leads to scaling of LWC and setting "Scale-NC" to the scaling of N(z).
Approach to calculate LWC(z) and N(z) is used as follows:
Case "Scale-WC"

LWC(z)

The program considers the second column in the file "cld_prof_inp.vin" as the shape of the LWC profile, $S_h(z)$. LWC(z) in absolute units is obtained multiplying shape profile by scaling factor: $C_f = \tau/[\int S_h(z)\, k_e(z)\, dz\,]$, where the integration is performed over a cloud layer, $k_e(z)$ is the extinction coefficient at 500 nm wavelength calculated for unity LWC and droplets effective radius $r_e(z)$ employing approximate formulas (Kokhanovsky, 2004a).

N(z)

N(z) in absolute units is obtained as follows: $N(z) = LWC(z)/\bar{V}(z)$, where $\bar{V}(z)$ is average volume of water droplets for a given effective radius profile $r_e(z)$.

Case "Scale-NC"

N(z)

The program considers the second column in the file "cld_prof_inp.vin" as the shape of the N(z) profile, $S_h(z)$. N(z) in absolute units is obtained multiplying shape profile by scaling factor: $C_N = \tau / [\int S_h(z)\, \sigma_e(z)\, dz\,]$, where the integration is performed over a cloud layer, $\sigma_e(z)$ is the extinction cross-section at 500 nm wavelength from available database interpolated at a given $r_e(z)$ profile.

LWC(z)

LWC(z) in absolute units is obtained as follows: LWC(z) = N(z) $\bar{V}(z)$, where $\bar{V}(z)$ is average volume of water droplets for a given effective radius profile $r_e(z)$.

"WATER_PATH"

A cloud layer is characterized by the liquid water path, LWP, which is defined by the second input value ("LWP" field) in the "Input integral parameter" control line, the first and two last fields in the same control line must be present but will not be used in the calculations (see example given above).

To obtain desired LWP the liquid water shape-profile will be scaled. Approach to calculate LWC(z) and N(z) is used as follows:

LWC(z)

The program considers the second column in the file "cld_prof_inp.vin" as the shape of the LWC profile, $S_h(z)$. LWC(z) in absolute units is obtained multiplying shape profile by scaling factor: $C_f = \text{LWP} / [\int S_h(z)\, dz\,]$, where the integration is performed over a cloud layer.

N(z)

N(z) in absolute units is obtained as follows: N(z) = LWC(z)/$\bar{V}(z)$, where $\bar{V}(z)$ is average volume of water droplets for a given effective radius profile $r_e(z)$.

"LWC_PROFILE"

A cloud layer is characterized by the liquid water concentration profile. Note that the control line "Input integral parameter" must always contains four input values, although in this case non of them will be used in the calculations.

Approach to calculate LWC(z) and N(z) is used as follows:

LWC(z)

The program considers the second column in the file "cld_prof_inp.vin" as the LWC profile in absolute units [g/m^3].

N(z)

N(z) in absolute units is obtained as follows: N(z) = LWC(z)/$\bar{V}(z)$, where $\bar{V}(z)$ is average volume of water droplets for a given effective radius profile $r_e(z)$.

"DENS_PROFILE"

A cloud layer is characterized by the vertical profile of water droplet density, N(z). Note that the control line "Input integral parameter" must always contains four input values, although in this case non of them will be used in the calculations.

Approach to calculate LWC(z) and N(z) is used as follows:

LWC(z)	N(z)
LWC(z) in absolute units is obtained as follows: LWC(z) = N(z)$\bar{V}(z)$, where $\bar{V}(z)$ is average volume of water droplets for a given effective radius profile $r_e(z)$.	The program considers the second column in the file "cld_prof_inp.vin" as the N(z) profile in absolute units [1/cm^3].

Attention:

- The average volume of water droplets, $\bar{V}(z)$, will be calculated automatically by the program;
- The shape profile, $S_h(z)$, will be set automatically by the program to an arbitrary constant for a vertically homogeneous cloud layer, i.e., if control parameter "Cloud layers are vertically inhomogeneous" is set to "no";
- The vertical profile $r_e(z)$ is used as third column in the file "cld_prof_inp.vin" or as constant defined in "Cloud particle geometrical dimension" input line of the file "cloud.inp";
- The options "LWC_PROFILE" and "DENS_PROFILE" can be used if parameter "Cloud layers are vertically inhomogeneous" is set to "yes".

3.15.3 Ice clouds: "Type of input integral parameter"

Appropriate control file: "cloud.inp"
Relevant control parameters: "Input integral parameter"

"TAU"
A cloud layer is characterized by its optical thickness, τ, at the wavelength 500 nm. Although the optical thickness is defined by the third entry ("TAU" field) in the "Input integral parameter" control line, three additional input entries must be given in the same control line, even though they will not be used in the calculations (see example below).

```
## ---------------------------------------
## |                                     |
## |----  Water ------|------  Ice -----|
## |  TAU   |    LWP  |    TAU  |   IWP |
##
Input integral parameter
     20.0      42.477     1.0     8.431
## ---------------------------------------
```

To obtain desired optical thickness of an ice cloud the ice water content shape-profile will be scaled. (In contrast to the water cloud the alternative scaling of N(z) profile was not implemented yet.) Approach to calculate ice water content IWC(z) and N(z) is used as follows:

IWC(z)	N(z)
The program considers the fourth column in the file "cld_prof_inp.vin" as the shape of the IWC profile, $S_h(z)$. IWC(z) in absolute units is obtained multiplying shape profile by scaling factor: $C_f = \tau/[\int S_h(z)\, k_e(z)\, dz\,]$, where the integration is performed over a cloud layer, $k_e(z)$ is the extinction coefficient at 500 nm wavelength calculated for unity IWC and corresponding effective radius $r_e(z)$.	N(z) in absolute units is obtained as follows: $N(z) = IWC(z)/\bar{V}(z)$, where $\bar{V}(z)$ is average volume of a hexagonal prism or fractal ice particles.

Attention:

- In the case of fractal and hexagonal prism extinction coefficient $k_e(z)$ is calculated employing approximate formulas (Kokhanovsky, 2004a). The effective radius of ice crystals is calculated for a given form of ice crystal as $r_e = 3\bar{V}/\bar{S}$, where $\bar{V}$ and $\bar{S}$ are the average volume and average area, respectively.
- In the case of Baum database $k_e(z)$ is pre-calculated and given within database, r_e is the seventh column in the file "cld_prof_inp.vin". k

"WATER_PATH"

A cloud layer is characterized by the ice water path, IWP, which is defined by the fourth input value ("IWP" field) in the "Input integral parameter" control line, the first three fields in the same control line must also be present, although they will not be used in the calculations (see example given above).

Approach to calculate IWC(z) and N(z) is used as follows:

IWC(z)	N(z)
The program considers the fourth column in the file "cld_prof_inp.vin" as the shape of the IWC profile, $S_h(z)$. IWC(z) in absolute units is obtained multiplying shape profile by scaling factor: $C_f = IWP/[\int S_h(z)\, dz\,]$, where the integration is performed over a cloud layer.	N(z) in absolute units is obtained as follows: $N(z) = IWC(z)/\bar{V}(z)$, where $\bar{V}(z)$ is average volume of a hexagonal prism or fractal ice particles.

"IWC_PROFILE"

A cloud layer is characterized by the ice water concentration profile. Note that the control line "Input integral parameter" must always contains four input values, although in this case non of them will be used in the calculations.

Approach to calculate IWC(z) and N(z) is used as follows:

IWC(z)	N(z)
The program considers the fourth column in the file "cld_prof_inp.vin" as the IWC profile in absolute units $[g/m^3]$.	N(z) in absolute units is obtained as follows: $N(z) = LWC(z)/\bar{V}(z)$, where $\bar{V}(z)$ is average volume of a hexagonal prism or fractal ice particles.

"DENS_PROFILE"
A cloud layer is characterized by the vertical profile of ice crystal density, N(z). Note that the control line "Input integral parameter" must always contains four input values, although in this case non of them will be used in the calculations.
Approach to calculate IWC(z) and N(z) is used as follows:

IWC(z)	N(z)
IWC(z) in absolute units is obtained as follows: IWC(z) = ρ N(z)$\bar{V}(z)$, where ρ and $\bar{V}(z)$ are the ice density and average volume of hexagonal prism or fractal ice particles, respectively.	The program considers the fourth column in the file "cld_prof_inp.vin" as the N(z) profile in absolute units $[1/cm^3]$.

Attention:

- The options "IWC_PROFILE" and "DENS_PROFILE" can be used if parameter "Cloud layers are vertically inhomogeneous" is set to "yes".
- The average volume of ice crystals, $\bar{V}(z)$, will be calculated automatically by the program or read from file in the case of Yang database;
- The shape profile, $S_h(z)$, will automatically be set by the program to a constant (unity) for a vertically homogeneous cloud layer, i.e., if control parameter "Cloud layers are vertically inhomogeneous" is set to "no";
- The vertical profiles of side length of hexagonal prism and edge length of regular tetrahedron are used as fifth and seventh columns in the file "cld_prof_inp.vin" or as constant defined in "Cloud particle geometrical dimension" input line of the file "cloud.inp" (height of hexagonal prism can be set to 100 μm only);

3.15.4 Mixed clouds (ice/water mixture)

Appropriate control file: "cloud.inp"
Relevant control parameters: "Expansion coefficients input file", "Input integral parameter"

The mixed cloud is considered as a composition of water droplets and ice crystals. Therefore, the mixed cloud can be installed following recommendations given above for the water and ice clouds. A mixed cloud can be modeled setting in the "Thermodynamic state" control line "mixed" (see above).

3.15.5 Additional absorber within a cloud/snow layer

Appropriate control file: "cloud.inp"
Relevant control parameters: "Additional absorber within cloud", "Wavelength grid for absorbers in cloud", "Real and imaginary part of refractive index",
"Relative concentration of absorber"

An additional absorber (e.g., soot or an another pollutant) can be introduced within each cloud or snow layer. This option can be used, e.g., to model impurities within a snow layer. If one set "t" in "Additional absorber within cloud" input line, the following input parameters have to be defined:

- the "Wavelength grid for absorbers in cloud" input line defines the wavelength grid [nm] in the ascending order, where optical properties of an absorber will be given;
- the "Real and imaginary part of refractive index" input line has the following structure:

```
#      It has to be defined for each cloud layer
#  first wl   |   second wl    |  .....
#  Re    Im   |  Re      Im    |  .....
Real and imaginary part of refractive index
1.34  0.44     1.34  0.44
1.34  0.44     1.34  0.44
```

  The first and second input lines contain refractive indices of absorber in the lower and upper cloud layer, respectively. The refractive index will be used to calculate absorption coefficient of a given absorber;
- the "Relative concentration of absorber" input line supplies the concentration profile within all cloud layers. The structure of input field is given in the following example in the case of two cloud layers:

```
##   Volume absorber concentration [m^3/m^3] within cloud layers
##   !! The number of levels (N), where concentration is defined !!
##   !!         has to be the same for all layers                 !!
##   First layer:
##   ---------------------------------------------------
##    line 1    :    altitude_1 |   concentration_1
##   ...............     ..........       ............
##    line N     :    altitude_N |   concentration_N
##   ---------------------------------------------------
##   Second layer:
##   ---------------------------------------------------
##    line 1    :    altitude_1 |   concentration_1
##   ...............     ..........       ............
##    line N     :    altitude_N |   concentration_N
##   ---------------------------------------------------
##         altitude is dimensionless height [0,1] from the cloud top
##             to the cloud bottom: (z_top - z)/(z_top - z_base)
##   Altitude and concentration have to be defined for each cloud layer
Relative concentration of absorber
0.0    1.0e-11
0.5    1.0e-11
1.0    1.0e-11
0.0    1.0e-10
0.5    1.0e-10
1.0    1.0e-10
```

3.15.6 Cloud as aerosol layer

Setting the control parameter "Thermodynamic state" to "alay", one can consider an aerosol cloud, i.e., a cloud as an aerosol layer consisting of aerosol particles but not from water particles or ice crystals.
The number and position of aerosol layers are defined using "Number of cloud layers" and "Cloud layer base and top" input lines similar to the case of water or ice cloud. The number of sub-layers within each aerosol layer is controlled by "Cloud sub-layers number" input field. This number depends on the vertical inhomogeneity of an aerosol layer and has to be ≥ 2. It is recommended to increase the number of sub-layers if calculation should be performed within gaseous absorption bands like O_2-A, O_2-B, H_2O, CO_2, etc.
Limitations: Only one aerosol layer is allowed (preliminary restriction).

The shape profiles of aerosol particles number density within aerosol layer should be specified setting the "Cloud layers are vertically inhomogeneous" parameter to "yes". The information about the vertical profile of aerosol particels density within layer has to be given in a separate file. Parameter "Cloud particle profile input file" defines the corresponding file name. The structure of this file is explained in Sec. 3.15.1 (see Example of the file structure "cld_prof_inp.vin"). In the case of cloud as aerosol layer two first columns in this file will be used only. Other columns in this file have to be given but will not be used by the program.

The scattering functions/matrices, scattering and extinction cross-sections of aerosol layer can be introduced setting in the "Phase function of cloud layers" input line "user". In this case the program will read scattering, extinction cross-sections, and scattering function/matrix moments as well as the wavelength grid from the user-defined files in the "Expansion coefficients input file" input line. The "Expansion coefficients input file" control line consist of two entries:

```
Expansion coefficients input file
'aer_wl_grid.dat'  'phm_names.dat'
```

first entry is the filename of file ("aer_wl_grid.dat") containing the wavelength grid on which optical parameters of aerosol layer will be given;

```
*  Example of the file 'aer_wl_grid.dat' containing the wavelength grid.
#   First line       - number of wavelengths
#   Subsequent lines - wavelength in [nm]
 2
750.0
780.0
```

second entry is the filename of the file ("phm_names.dat") having the following structure:

```
#   fist line after auxiliary symbol ">" contains
#         filename with the extinction cross-section at a reference
#         wavelength;
#   other lines - filenames containing scattering functions/matrices and
```

```
#         extinction/scattering cross-sections at the wavelength grid
#         given in the file "aer_wl_grid.dat".
#         Number of other lines has to be equal to the number of wavelengths
#         in the file given above.
>
 '../data/aerosol/aer_ref_ecs.dat'
 '../data/aerosol/hg_g07_ssa1.dat'
 '../data/aerosol/hg_g07_ssa1.dat'
```

The structure of the file containing extinction cross-section at a reference wavelength is given as follows:

```
#     An extinction cross-section [micron^2] at reference wavelength.
#
    0.168901251464155D+03
```

The structure of the file containing scattering functions/matrices ("hg_g07_ssa1.dat") is the same as in the case of cloud if the option "user" is selected in "Phase function of cloud layers" input line (see detailed explanation in "Select scattering function/matrix and scattering, extinction cross-sections of cloud layer").
The control parameter "Use constant phase function within cloud layer" has to be set to "t". The control parameter "Delta-M or Delta-Fit" has to be set to "D-M", and the parameter "Delta-m truncation for cloud layers" has to be set to $N_{LM} - 1$, where N_{LM} is the number of Legendre moments as defined in "control_ac.inp" control file.

As an input integral parameter of aerosol layer only option "TAU" in the "Type of input integral parameter" input line can be selected. The desired value of the optical thickness (τ_a) should be given in the first entry of the "Input integral parameter" control line. This optical thickness will be considered by program as the optical thickness at reference wavelength and used to calculate particles number density profile

$$N(z) \;=\; S_h(z)\,\frac{\tau_a}{\sigma_e \int S_h(z)\,dz}\;, \tag{3.13}$$

where the integration is performed over an aerosol layer, σ_e is the extinction cross-section at reference wavelength as give in the file "aer_ref_ecs.dat", and $S_h(z)$ is the shape profile as defined in the second column of the file "cld_prof_inp.vin".
The extinction coefficient vertical profile at all discrete wavelengths (λ_i) given in the file "aer_wl_grid.dat" will be calculated as follows:

$$k_e(z,\lambda_i) \;=\; N(z)\,\sigma_e(\lambda_i)\;, \tag{3.14}$$

where $\sigma_e(\lambda_i)$ is the extinction cross-section as given in the file containing scattering functions/matrices, e.g., "hg_g07_ssa1.dat".
Limitations:
The single scattering albedo ($\sigma_s(\lambda_i)/\sigma_e(\lambda_i)$) and scattering function/matrix are assumed to be constant within aerosol layer.

The following input parameters presented in the "cloud.inp" control file are irrelevant for the option "alay":

"Cloud particle geometrical dimension", "Filenames in database",
"Form of ice crystals", "Lower and upper value of forward cone",
"Path to cloud data bases", "Refractive index of water and ice",
"Scattering and absorption coefficients", "Will be scaled vertical profile of"

3.16 Surface reflection

Appropriate control files: "control.inp", "control_brdf.inp"
Relevant control parameters: "Surface reflection type", "Albedo", "Path to the albedo database", "Spectral albedo filename", "Replacement for water"

3.16.1 General

The user can switch between different options to take into account surface reflection in the radiative transfer calculations. One can set in the "Surface reflection type" input line the following keywords: "alb_const", "alb_spec", "alb_db_mts", and "brdf". They will be interpreted by the program as follows:

- "alb_const" - independent of the wavelength Lambertian reflection.
  A constant albedo for a Lambertian surface is set in the "Albedo" input line.
- "alb_spec" - wavelength dependent Lambertian reflection.
  A wavelength dependent Lambertian albedo from the spectral database is used instead of a constant value. The path to the database and the filename should be specified in the "Path to the albedo database" and "Spectral albedo filename" input lines, respectively. The input field of "Spectral albedo filename" input line consists of two entries:
  first entry - file name,
  second entry - the number of columns (N_A) linear combination of which will be used to calculate surface albedo. If $N_A > 1$ then in the "Weights of albedo components" input line should be given weights of albedo components. The surface albedo will be calculated by the program as follows:

$$A = \sum_{i=1}^{N_A} W_i A_i , \tag{3.15}$$

  where W_i and A_i are weights and albedo of selected components, respectively.
  A desired surface type is selected specifying an appropriate name for the spectral database. The following databases are available:
  albedo_rg_sand.dat, albedo_rg_soil.dat, albedo_rg_water.dat,
  albedo_rg_snow.dat, albedo_rg_vegetation.dat .
  The file structure should be as follows. After header lines (each line at the beginning of file containing any character except of $0, 1, \ldots, 9, E, e, D, d$ will be considered as a comment line) follows the line containing the number of spectral points in the file. Following lines consist of two entry: first entry wavelength in [nm], second entry - albedo. Wavelengths should be given in ascending order.
  Limitation: This database is available in the spectral range 240 - 800 nm only.

Attention: The file containing the spectral albedo for different surface components should be provided by user.

- "brdf" - bidirectional reflectance distribution function.
  A non-Lambertian surface reflection can be modeled using an appropriate parameterization for the bidirectional reflectance distribution function (BRDF) (Lyapustin, 1999; Pinty et al., 2000; Degünther and Meerkötter, 2000; Cox and Munk, 1954a). A desired surface type is selected in the "Surface type" control line ("control_brdf.inp" file).

3.16.2 Bidirectional reflectance distribution functions (BRDF)

Appropriate control files: "control_brdf.inp"
Relevant control parameters:
"Surface type", "BRDF output control", "Output of spherical albedo", "Exact BRDF for diffuse radiation"

The user can switch between numerous BRDF models describing a land and ocean reflectance using the "Surface type" control parameter input line.

Land reflectance is presented by the following models (see Sect. 3.16.2.1):
RPV model and modified RPV model;
Kernel-based Ross-Li vegetation-soil model;
Kernel-based Ross-Li standard MODIS BRDF model;
modified RPV plus facet model;
reflectance of canopy layer using incorporated PRO4SAIL code.

Ocean reflectance is presented by the following models (see Sect. 3.16.2.2):
- Fresnel reflectance from the flat or wind-roughed air-water interface;
- whitecaps reflectance;
- water leaving reflectance.

The user can supply own routine to calculate BRDF (see Sect. 3.16.2.3).

Independent of the selected reflectance model the following options can be used.

Enhanced accuracy mode.
Setting in the "Exact BRDF for diffuse radiation" control line "t" the user forces the program to calculate reflected by the surface diffuse radiation using exact values of BRDF. If this control parameter is set to "f" then BRDF at the user-defined directions of observation will be obtained using interpolation between Gaussian quadrature nodes.
Limitation: This option is irrelevant if the "RTM_TYPE" control parameter is set to "spher_scat".
Attention: This option can be time consuming if BRDF should be calculated at larger amount of wavelengths.

Output of spherical albedo.
The spherical albedo (an integral parameter of BRDF) will be calculated and written out as output parameter in the "SCE_SUMMARY.OUT" output file located in the directory "./DATA_OUT". This option will be active if the first entry in the "Output of spherical albedo" control line is greater than "0". The first entry will be interpreted by the program as

the number of wavelength where spherical albedo should be calculated. The following entries will be considered as output wavelengths in [nm].

Output of BRDF in separate file.
The used by the program BRDF can be written out for the visual representation in output file. BRDF is written out for the first wavelength and first solar zenith angle. The program generates this file if the user set "t" in the "BRDF output control" input line. The second input line contains the output-filename including path. The file consists of the header and BRDF for the discrete number of the zenith and azimuthal angles. The details of the file structure is described in the file header.

3.16.2.1 Land surface reflection

Appropriate control files: "control_brdf.inp"
Relevant control parameters:
"Surface type", "BRDF spectral range", "Spherical albedo of vegetation and soil", "Vegetation fraction", "Hot spot parameter", "Extrapolation type of Ross-Li model", "Extrapolation type of svk model", "Coefficients of Ross-Li BRDF model"

The following settings in the "Surface type" control line are supported:

RPV model proposed by Rahman et al. (Rahman et al., 1993)
"spruce", "sparse erectophile", "tropical forest", "plowed field", "grasses", "broad leaf crops", "Savannah", "leaf forest", "Conifers", "hardwood forest winter", "loam soil", "irrigated wheat", "dark", "bright"

For these surface types two different set of parameters, i.e., for UV and near-IR spectral ranges are available. A desired spectral range is selected setting "BRDF spectral range" parameter to "UV" or "IR".

Modified RPV model (Degünther and Meerkötter, 2000) : "snow"

The parameters for snow reflection model is available in the UV spectral range only.

Kernel-based Ross-Li vegetation-soil model : "svk"

This BRDF model allows to simulate not only directional but also spectral dependence of the surface refection. The user should define the following input parameters:

- two entries of "Spherical albedo of vegetation and soil" input parameter contains filenames (including path) which comprise the spherical albedo of vegetation and soil as a function of wavelength. The file-structure is the same as described above for the option "alb_spec";
- the input parameter "Vegetation fraction" contains the desired fraction of vegetation in the mixture vegetation-soil;
- the input parameter "Hot spot parameter" contains the hot spot parameter. Recommended value is in the range 1-2°.
- the "Extrapolation type of svk model" control parameter defines extrapolation type of the kernel-based BRDF at zenith angles ϑ larger than ϑ_{max}. Tne first entry of this control line defines the extrapolation type:
  "off" - BRDF will be used according to the selected model at all ϑ;

"zero" - BRDF values will be set to zero at $\vartheta > \vartheta_{max}$;
"const" - BRDF values will be set to BRDF(ϑ_{max}) at $\vartheta > \vartheta_{max}$.
Tne second entry of this control line defines ϑ_{max} in [°].
Note that this option can be used to avoid not physical values of some BRDF parameterizations at large incidence and reflection angles.

Kernel-based Ross-Li standard MODIS BRDF model ": Ross-Li"

This BRDF model allows to simulate the directional and spectral dependences of the surface refection using the wavelength dependent coefficients of Ross-Li standard MODIS BRDF model given as

$$R(\mu_v, \mu_s, \varphi_r; \lambda_i) \;=\; f_{\rm iso}(\lambda_i) \;+\; f_{\rm vol}(\lambda_i)\, K_{\rm vol}(\mu_v, \mu_s, \varphi_r) \;+\; f_{\rm geo}(\lambda_i)\, K_{\rm geo}(\mu_v, \mu_s, \varphi_r)\;. \quad (3.16)$$

The details of representation functions $K_{\rm vol}$ and $K_{\rm geo}$ are given in (Rozanov et al., 2014).
The user should define the following input parameters:

- the "Coefficients of Ross-Li BRDF model" input parameter contains filename (including path) of the file comprising coefficients $\{f_{\rm iso}(\lambda_i), f_{\rm vol}(\lambda_i), f_{\rm geo}(\lambda_i)\}$ at discrete number of wavelengths. The file-structure is as follows:
  - each line at the beginning of the file containing any character except of $0, 1, \ldots, 9, E, e, D, d$ will be considered as a comment line (header block);
  - the first line after header block contains the number of wavelengths N_λ, for which coefficients $\{f_{\rm iso}(\lambda_i), f_{\rm vol}(\lambda_i), f_{\rm geo}(\lambda_i)\}$ are given;
  - the following N_λ lines consist of four columns, i.e., first column contains wavelength grid in [nm] in ascending order, and following three column contain coefficients $\{f_{\rm iso}(\lambda_i), f_{\rm vol}(\lambda_i), f_{\rm geo}(\lambda_i)\}$.
- the "Extrapolation type of Ross-Li model" control parameter defines extrapolation type of the kernel-based BRDF at zenith angles ϑ larger than ϑ_{max}. Tne first entry of this control line defines the extrapolation type:
  "off" - BRDF will be used according to the selected model at all ϑ;
  "zero" - BRDF values will be set to zero at $\vartheta > \vartheta_{max}$;
  "const" - BRDF values will be set to BRDF(ϑ_{max}) at $\vartheta > \vartheta_{max}$.
  Tne second entry of this control line defines ϑ_{max} in [°].
  Note that this option can be used to avoid not physical values of this BRDF parameterization at large incidence and reflection angles.

Modified RPV plus facet model: "mRPV_facet"

This BRDF model represents the surface reflectance as a sum of two components, i.e.,
1) a volumetric scattering term that is completely depolarizing and
2) a specular reflection term.
The modified Rahman-Pinty-Verstraete (mRPV) function (excluding the hotspot correction) is used for the volumetric term:

$$R_1 \;=\; \frac{a_\lambda}{\pi}[(\mu+\mu_0)\mu\mu_0]^{k-1}\, e^{-b\cos\gamma}\;, \quad (3.17)$$

where a_λ, k, and b are input parameters, γ is the scattering angle.
Second component is polarized and it represents the facet reflection like Cox and Munk ocean

reflection model:

$$R_2 \;=\; \zeta \,\frac{\mathcal{P}(\mu_n)\, S(\mu,\mu_0)}{4\mu\mu_0\mu_n}\, \mathbf{L}(-\alpha)\, \mathbf{F}(\gamma, m_r, m_i)\, \mathbf{L}(\alpha_0)\;, \tag{3.18}$$

where ζ is a scaling parameter which defines the contribution of this component in the total reflection, $\mathcal{P}(\mu_n)$ is the facet slope probability distribution function, $S(\mu,\mu_0)$ is the shadowing factor, $\mathbf{L}(-\alpha)$ and $\mathbf{L}(\alpha_0)$ are rotation matrices, $\mathbf{F}(\gamma, m_r, m_i)$ if the Fresnel reflection matrix depending on the real m_r and imaginary m_i part of the surface refractive index.

The user should define the following model parameters: a_λ, k, b and ζ, m_r, m_i. It can be done using the following control parameter:

- the "Filename (including path) containing model parameters" control line contains filename of the file comprising model parameters listed above. An example of the file is given as

```
#          This is a file structure containing a parameters
#               of mixed (mRPV + facet) BRDF model
#                  including polarization
#          column
#              1   wavelength in [nm]
#              2-4 parameters of modified RPV model  (a, k, b)
#              5-7 parameters of micro-facet
#              5 - scaling parameter,
#              6 - real part of refractive index
#              7 - imaginary part of refractive index
# 1      2      3      4        5      6     7
#        <---- mRPV ---->      <----- facet ---->
#         a      k      b              re     im
 470.   0.2     1.    0.       1.0    1.5   0.0
 660.   0.2     1.    0.       1.0    1.5   0.0
```

  All lines beginning with # are header lines. First column in this file contains the wavelength grid in ascending order where corresponding model parameters are defined.
- The "The slope variance" control parameter contains the slope variance of the Gaussian facet distribution function.
  Note that if the slope variance is set to 0 then instead of Gaussian PDF will be used Breon's PDF Breón et al. (1995) and corresponding shadowing factor, i.e.,

$$\mathcal{P}(\mu_n) = \frac{\mu_n}{\pi}\;, \qquad S(\mu,\mu_0) = \frac{2\mu\mu_0}{\mu+\mu_0}\;. \tag{3.19}$$

- If the "Use shadowing factor?" control parameter is set to "yes" then the shadowing effects with the appropriate shadowing factor will be accounted for.

Reflection of canopy layer using incorporated PRO4SAIL code: "prosail"

BRDF of canopy layer will be calculated in this case using incorporated into SCIATRAN model the PRO4SAIL code. The following settings is relevant if "Surface type" control parameter is set to "prosail" :

```
## ********************************************************************
```

```
##     Leaf inclination distribution function type and parameters
##     Type = 1 :
##          first parameter controls the average leaf slope
##          second parameter controls the distribution's bimodality
##        Parameters    a     b   requirement: |a| + |b| < 1
##        ----------------------
##        Planophile    1     0
##        Erectophile  -1     0
##        Plagiophile   0    -1
##        Extremophile  0     1
##        Spherical    -0.35 -0.15
##        Uniform       0     0
##        ----------------------
##      Type = 2 - ellipsoidal distribution. Parameters:
##         a - average leaf angle (degrees) (0 = planophile 90 = erectophile)
##        b = 0
##      ------------------------------------------------------------------------
## Type    a       b
Leaf inclination distribution function
    1    -0.35    -0.15

##     Other parameters of canopy layer
##         LAI    - leaf area index (m^2/m^2)
##         hspot  - hot spot parameter
##         Cab    - chlorophyll content (micro_gr/cm^2)
##         Car    - carotenoid content (micro_gr/cm^2)
##         Cbrown - brown pigment content (arbitrary units)
##         Cw     - EWT (cm)
##         Cm     - LMA (g/cm^2)
##         Stc    - structure coefficient
##         Psoil  - soil factor (psoil=0: wet soil / psoil=1: dry soil)
## LAI  hspot  Cab  Car  Cbrown   Cw    Cm     Stc  Psoil
Other parameters:
   3.     0.01    1.   8.   0.0    0.01  0.009   1.5    1.
## ------------------------------------------------------------------------
```

3.16.2.2 Ocean surface reflection

Appropriate control files: "control_brdf.inp"
Relevant control parameters:
"Absorption coefficients", "Absorption coefficients file name", "Absorption coefficients input type", "Angular scattering coefficient filename", "Diameter of bubbles", "Liquid fraction", "Mean square slope", "Peakedness and skewness coefficients", "Refractive index file name", "Refractive index input type", "Refractive index of water", "Replace cosine", "Seawater general properties", "Shadowing effects?", "Specular reflection", "Surface slope PDF", "Surface type", "Upwind and crosswind slopes", "Whitecaps Glint Water leaving"

Attention: The ocean surface reflection will be accounted for by the program if
- control parameter "Surface reflection type" in "control.inp" file is set to "brdf";
- control parameter "Surface type" in "control_brdf.inp" file is set to "ocean".

There are different options in SCIATRAN to describe reflection from the oceanic surface. In particular, the reflectance of an ocean surface can be calculated as the sum of three following component:

- the reflectance due the whitecaps (scalar case only);
- the Fresnel (specular) reflectance (scalar and vector);
- the reflectance emerging from the sea water so called water leaving reflectance (scalar case only).

The user can select one or more above mentioned reflectance components setting in the
```
Whitecaps      Glint      Water leaving
```
input field consisting of three entry, "off", "scalar" or "vector", excluding or including in the scalar/vector case corresponding component of the oceanic reflectance. The following combination is relevant in the existing SCIATRAN version:

- "Whitecaps" - "off"/"scalar";
- "Glint" - "off"/"scalar"/"vector";
- "Water leaving" - "off"/"scalar".

Thus, for example, according to the following input line:
```
Whitecaps      Glint      Water leaving
   off         vector       scalar
```
in the reflectance of the ocean surface contribute the Fresnel reflection and water leaving radiation in the vector and scalar form, respectively. The contribution of whitecaps is excluded.
Attention: The total oceanic reflection is calculated as follows:

$$R_{ocean} = c\,R_{WC} + (1-c)\,(R_{WL} + R_{Fr})\,, \tag{3.20}$$

where c is the fraction of surface covered by foam, R_{WC}, R_{Fr}, and R_{WL} are whitecaps, Fresnel, and water leaving reflectance, respectively. It is assumed that c is determined by the wind speed. In particular, the parameterization of Monahan and Muircheartaigh (Monahan and Muircheartaigh, 1981) is employed in SCIATRAN.

If the components which contribute in the total reflectance are defined, then the user should perform the following settings

- Set main properties of the seawater.
  The main properties of the seawater should be defined in the "Seawater general properties" input line. The input field consists of eight entries which have the following meaning:
  - 1 - Sea surface temperature [°C];
  - 2 - Salinity [g/kg];
  - 3 - Chlorophyll concentration [mg/m^3];
  - 4 - Concentration of small particles [ppm], [cm^3/m^3]. The small fraction represents terrigenous particles with density $\rho_s = 2$ g cm^{-3}, relative (to the water) refractive index $n_s = 1.15$, and the size distribution in the region [0.01,1.3] μm.
  - 5 - Concentration of larger particles [ppm], [cm^3/m^3]. The larger fraction represents organic particles of phytoplankton and detritus with the density of $\rho_l = 1$ g cm^{-3},

relative refractive index $n_s = 1.03$, and the size distribution in the region [1.3,13] μm.

- 6 - Model of the pure seawater volume scattering function according to "Morel", "Shifrin" or "Buiteveld";
- 7 - Wind speed at 10 m above surface [m/s];
- 8 - Azimuthal angle of the upwind direction relative to the direction of solar light [deg].
  Note that this parameter will be only used if the "Surface slope PDF" input line is set to "Gram-Charlier" (see below).

- Set parameters for Fresnel reflection (option "Glint").
  The probability distribution function (PDF) of the surface slope can be used setting in the "Surface slope PDF" input line "Gauss" or "Gram-Charlier".
  "Gauss" PDF.
  If control parameter "Surface slope PDF" is set to "Gauss", then the mean square slope σ^2 of the Gaussian probability distribution function has to be defined in the "Mean square slope" input line. The input field consists of two entries. They are parameters in the following approximation of σ^2:

$$\sigma^2 = A + B \cdot V \,, \tag{3.21}$$

  where V is the wind speed (the seventh entry in the "Seawater general properties" input line), A and B are the first and second entries in the "Mean square slope" input line.
  "Gram-Charlier" PDF.
  If control parameter "Surface slope PDF" is set to "Gram-Charlier", the program needs the input of following parameters:
  - The "Peakedness and skewness coefficients" input line should be used to define peakedness and skewness coefficients and their dependence on the wind speed in the Gram-Charlier PDF. Setting in this input line "Cox_Munk" or "Breon_Henriot", the user can switch between approximation given by Cox and Munk (Cox and Munk, 1954b) or Breon and Henriot (Breón and Henriot, 2006), respectively.
  - The "Upwind and crosswind slopes" input line should be used to define in which form the upwind and crosswind mean square slope are introduced below.
    Setting in this input line "coeff" or "ratio", the user can switch between two option to input upwind and crosswind mean square slope:

"coeff"	"ratio"

The upwind and crosswind mean square slope are given in the form of Eq. (3.21). The parameters A_u, B_u, A_c, and B_c should be given in the "Mean square slope" input line along with parameters A and B as follows:
`Mean square slope`
`A B Au Bu Ac Bc`
	The input parameter to define upwind and crosswind mean square slope is the ratio σ_u^2/σ_c^2. The σ_u^2 and σ_c^2 square slope will be calculated by the program using additionally the following relation: $\sigma_u^2 + \sigma_c^2 = \sigma^2$. The "Mean square slope" input line consists in this case of three entries:
	A B σ_u^2/σ_c^2

Attention:

- Two first entries in the "Mean square slope" input line contains always linear regression parameters A and B describing mean square slope σ^2 (see Eq. (3.21)). The additional one or four entries will be used by the program if the "Surface slope PDF" control parameter is set to "Gram-Charlier".
- The Gram-Charlier PDF is used by the program to calculate reflection of direct solar light. The reflection of diffuse radiation is calculated using Gaussian PDF.

Refractive index of water.
The calculation of the Fresnel reflection coefficient requires the refractive index of water. Setting in the "Refractive index input type" control parameter "const" or "wl_dep", the user can switch between usage of constant or wavelength dependent refractive index.

"const"	"wl_dep"
The real and imaginary part of the water refractive index should be given in the "Refractive index of water" input line.	The name of the file containing wavelength depended real and imaginary part of the water refractive index should be given in the "Refractive index file name" input line.

Attention: The file containing the refractive index consists of a header and three columns. Each line at the beginning of the file containing any character except of $0, 1, \ldots, 9$, E, e, D, d will be considered as a comment line.
First column contains wavelength in ascending order expressed in [μm].
Second and third columns contain real and imaginary part of the refractive index, respectively.
Shadowing effects of ocean waves.
The shadowing effects can be included or excluded setting in the "Shadowing effects?" input line, "yes" or "no", respectively.

- Set parameters for water leaving reflection (option "Water leaving").

The water leaving radiance is calculated in SCIATRAN using the modified Gordon approximation. The user needs to introduce following input parameters:
Scattering function of the seawater.
The name of the file containing the water angular scattering coefficient should be given in the "Angular scattering coefficient filename" input line. The file containing the angular scattering coefficient consists of a header and two columns.
Each line at the beginning of this file containing any character except of $0, 1, \ldots, 9$, E, e, D, d will be considered as a comment line.
First column contains the scattering angle in ascending order expressed in [deg].
Second column contains total angular scattering function in [m^{-1} ster^{-1}].
Absorption coefficients.
Setting in the "Absorption coefficients input type" control parameter "const" or "wl_dep", the user can switch between usage of constant or wavelength dependent absorption coefficients.

"const"	"wl_dep"
The absorption coefficients should be given in the "Absorption coefficients" input line. This input line consists of three entries: first entry is the absorption coefficient of the pure water [m^{-1}] at the reference wavelength 440 nm; second and third entries are absorption coefficients [m^{-1}] of the pure water and chlorophyll at the desired wavelength.	The name of the file containing wavelength depended absorption coefficients should be given in the "Absorption coefficients file name" input line. The file containing absorption coefficients consists of a header and three columns. Each line at the beginning of this file containing any character except of $0, 1, \ldots, 9$, E, e, D, d will be considered as a comment line. First column contains the wavelength in the ascending order expressed in [nm]. Second and third columns contain pure water and chlorophyll absorption coefficients, respectively, expressed in [m^{-1}].

- Set parameters for whitecaps reflection (option "Whitecaps").
  The whitecaps reflection is implemented in SCIATRAN according to an approximate model proposed in (Kokhanovsky, 2004b). The user should define liquid fraction of foam and diameter of bubbles in [mm] (typical range 0.1 - 1 mm). It can be done using the "Liquid fraction" and "Diameter of bubbles" input lines, respectively. The spectral absorption coefficient will be used by the program as defined in the option "Water leaving" reflectance.

3.16.2.3 User-defined surface reflection

Appropriate control files: "control_brdf.inp"
Relevant control parameters: "Surface type", "Number of wavelength for BRDF"

The user can define surface reflection properties with the help of any analytical approximation. For this purpose one needs to set in the "Surface type" input line "user" and adjusts the Fortran subroutine "user_brdf.f". The existing version of this routine contains the program code for calculation of the surface BRDF in the form of RPV approximation as proposed by Rahman et al. (Rahman et al., 1993).
Using this option, the user can define the surface BRDF as a function of the wavelength. The number of wavelengths should be given in the "Number of wavelength for BRDF" input line. The wavelengths grid should be defined in the "user_brdf.f" routine.

Limitation: This option can not be used along with the single scattering correction technique (see Section 3.7.5).

3.17 User-defined land fluorescence spectrum

Appropriate control file: "control.inp"
Relevant control parameters: "Include land fluorescence"

This option allows the user to include in radiative transfer calculation the fluorescence of vegetation in the form of an emission spectrum. This spectrum will be considered by the program as an emission source located at the lower boundary. The input field of "Include land fluorescence" parameter consists of many entries. The interpretation of the input field by the program depends on the first entry. There are three possibilities to set first entry:

- "off" - the radiative transfer calculations do not include the land vegetation fluorescence. All further entries in this input line will be ignored;
- "file" - the fluorescence spectrum should be provided by user in a separate input file;
- "Double-Gaussian" - the fluorescence spectrum will be calculated as a sum of two Gaussian distribution.

In the following we consider the structure of the "Include land fluorescence" parameter in the case if the first entry is set to "file" or to "Double-Gaussian".

The first entry of "Include land fluorescence" is set to "file"

The second entry will be interpreted by the program as a filename (including path) of the required emission spectrum, and third one as a scaling factor. The file containing an emission spectrum should be formatted as follows:

```
# fluorescence emission spectrum of velvegrass at canopy level (Rascher 2009)
# the spectrum have been scaled to a maximum value of 3.0 mW/m2/sr/nm
# wavelength in nm
# emission (top of canopy) in mW/m2/sr/nm
# wavelength   emission
  660.00000    0.34532
  660.09998    0.34587
  660.20001    0.34647
  660.29999    0.34709
  660.40002    0.34772
  660.50000    0.34837
```

In this example first 5 lines will be considered by program as comment lines. In fact the number of comment lines in the file header is arbitrary. Each line containing any character except of $0, 1, \ldots, 9, E, e, D, d$ will be considered as a comment line. The number of lines in the data block corresponds to the number of wavelengths (only six lines is shown in the example above). First column contains wavelength in [nm], second one the emission spectrum. The emission spectrum has to be given in [mW/m^2/nm/sr]. The scaling factor should be positive. The input spectrum will be multiplied by the program by this scaling factor.

The first entry of "Include land fluorescence" is set to "Double-Gaussian"

The following 6 entries provide parameters of Gaussian functions
$a_1,\ \lambda_1,\ s_1,\ \ a_2,\ \lambda_2,\ s_2$
where a is amplitude, λ is position of maximum [nm], and s is half width at half maximum

[nm]. Amplitudes have to be given in [mW/m^2/nm/sr]. The fluorescence spectrum will be calculated as

$$F(\lambda) \;=\; \sum_{i=1}^{2} a_i \exp\left[-\ln 2 \left(\frac{\lambda-\lambda_i}{\sigma_i}\right)^2\right] \tag{3.22}$$

Attention:

- The appropriate extra-terrestrial solar spectrum has to be used in absolute units, i.e., in the input line "Extra-terrestrial solar flux" should be set "File" (see Sec. 3.2).
- It is assumed that fluorescence spectrum is unpolarized and isotropical.
- The weighting function for the scaling parameter as well as for all parameters of Double-Gaussian fluorescence spectrum can be calculated (see Sec. 3.1.6).

Limitations. This mode can not be used if:

- control parameter "RTM_TYPE" is set to "spher_scat" (see Sec. 3.4.4);
- coupled ocean-atmosphere model is used (see Sec. 3.20);
- control parameter "RTM-CORE" is set to "CDI" (see Sec. 3.6.1).

3.18 Date and geolocation

Appropriate control file: "control.inp"
Relevant control parameters: "Date", "Latitude & longitude"

All parameters discussed in this section are needed to select an appropriate ozone vertical distribution from the selected climatological data base if "Ozone climatology" input parameter is set to any supported value other then "NONE"(see Section 3.12.2.4).

Set the date.
An appropriate date can be selected in "Date" control line. The first line below the keyword specify if a day of year ("DOY" mode) or date ("DMY" mode) will be set. The subsequent line must contain the number of day in the year (1 means January 1st) and year in "DOY" mode or date in "DD.MM.YYYY" format which will be read as string in "DMY" mode.

Set the geolocation.
To define the geolocation for the radiative transfer modeling, the input field "Latitude & longitude" is used, which contains two comma or space separated input values defining the latitude and the longitude, respectively. The corresponding values must be specified in deg between -90.0 (South pole) to +90.0 (North pole) for the latitude and between 0.0 and 360.0 for the longitude.

3.19 Thermal emission

Appropriate control files: "control_te.inp"
Relevant control parameters:
"Accuracy of Planck function approximation", "Extra-terrestrial solar flux",

"Output in brightness temperature", "Planck output control", "Set solar flux", "Spectral integration of Planck function", "Surface temperature", "Switch off solar light"

Thermal emission is considered in the radiative transfer calculations if "Thermal emission" flag is set to "t" in the main control file "control.inp". There are the following options to install all relevant to the thermal emission parameters:

- Select daytime or nighttime.
  Setting the "Extra-terrestrial solar flux" input line to "0" or "1" user can switch between nighttime and daytime, respectively.
  If the "Extra-terrestrial solar flux" parameter set to "0" only thermal emission will be considered, i.e., the contribution of the solar light will be set to zero.
  If the "Extra-terrestrial solar flux" parameter set to "1" the solar light will be considered also. The solar irradiance at the top of atmosphere will be used as defined in "control.inp" main input file.

- Exclude solar light.
  Setting the "Switch off solar light" control parameter to "t" user forces the program to calcualte the radiative transfer of thermal radiation only. This option is the same as obtained setting the "Extra-terrestrial solar flux" control parameter to "0" but faster because the program does not perform calculations of the direct solar light and corresponding particular solutions.

- Set desired value of the extra-terrestrial solar flux.
  User can define any desidred value of the extra-terrestrial solar flux.

  If the first entry in the "Set solar flux" input line is set to "t" the second entry will be interpreted by the program as the iincident solar flux.
  Attention:

  - this option is relevant if "Extra-terrestrial solar flux" parameter is set to "1" (see above);

  - the dimension of the iincident solar flux is used as define in the "control.inp" in "Dimension of extra-terrestrial solar flux " input line.

- Set desired surface temperature.
  User needs to define the surface temperature. This allows to introduce an jump between the air and surface temperature. The surface temperature in [°K] is introduced in "Surface temperature" input line.

- Perform spectral integration of the Planck function.
  User can employ in radiative transfer calculation the monochromatic or spectral integrated Planck function.
  If first entry in "Spectral integration of Planck function" is set to "t" the second and third entries define the lower and upper boundaries of the integration interval in wavenumbers [cm^{-1}].
  If first entry in "Spectral integration of Planck function" is set to "f" the Planck function will be calculated by program at a given wavelength as defined in "control.inp" file.

- Accuracy of Planck function approximation.
  To obtain the particular solution of radiative transfer equation the Planck function as a function of optical depth is approximated as a series of exponential functions. The accuracy of this approximation in [%] should be define in "Accuracy of Planck function approximation" input line.
- Select output dimension of the intensity.
  Setting in the "Output in brightness temperature" input line "t" the intensity in output file will be presented in [°K], i.e., in the form of the brightness temperature.
- Output of exact and approximated Planck functions.
  If first entry in the "Planck output control" input line is set to "t" the second entry will be interpreted by program as output file name which contains exact and approximate Planck functions.

3.20 Ocean-atmosphere coupling mode

Appropriate control files: "control_uwt.inp"
Relevant settings and control parameters:

Air-water interface: "Flat or wind-roughed ocean surface",
"Mean square slope and wind speed", "Approximation of RT matrices"
Coupled ocean-atmosphere: "Coupling"
Depth grid in the ocean: "Depth grid file name", "Layering of ocean",
"Layers number", "Ocean depth", "Profile scenario file name"
Refractive index of water: "Refractive index input type",
"Refractive index file name", "Reference wavelength grid",
"Refractive index of water"
Absorption of natural water:
"Pure water absorption coefficients file name",
"File name for chlorophyll concentration",
"Chlorophyll absorption coefficients file name",
"Approximation of CDOM absorption",
"Concentrations of fulvic and humic acids" "Use additional absorber in water"
Scattering of pure seawater: "Pure seawater scattering function",
"Pure seawater depolarization ratio", "Depolarization ratio filename",
"Constant depolarization ratio", "Rayleigh optical thickness of water"
Hydrosol scattering: "Number of hydrosol models", "Hydrosol angular scattering"
Inelastic processes: "Inelastic processes wihtin water"
Streaming: "Number of streams in ocean", "Number of Legendre moments"
Ocean bottom: "Ocean bottom albedo"
Other: "Do Akima interpolation", "Output of water-leaving radiance",
"Perform calculation in two-layer slab"

The radiative transfer in the ocean-atmosphere system will be performed by SCIATRAN if the control parameter "Include radiative transfer within ocean or ice" is set to "ocean" in

the control file "control.inp". The additional parameters which should be defined to describe ocean-atmosphere interface and scattering and absorption of the radiation in the water will be discussed in this section.

- Ocean surface properties.
  The air-water interface in SCIATRAN can be considered as a flat (specular reflection) or wind-roughed (Gaussian PDF) surface. The user can switch between these two possibilities setting in the "Flat or wind-roughed ocean surface" control line "flat" or "roughed", respectively.
  If the case of wind-roughed surface is chosen, the user need to define parameters of Gaussian PDF describing the wave slopes and approximation for the reflection and transmission matrices which should be used by the program.
  - Mean square slope parameters of Gaussian wave slope PDF and wind speed should be defined in the "Mean square slope and wind speed" control line. This line consist of three entry's. First two entry's define coefficients (A, B) of the linear relationship between mean square slope and wind speed (U): $\sigma^2 = A + B \cdot U$, and third entry is the wind speed U expressed in [m/s].
  - Approximation of reflection and transmission (RT) matrices in the case of rough ocean-atmosphere interface can be defined setting in the "Approximation of RT matrices" control line:
    - "SS" - single scattering approximation of RT matrices as used by Nakagjima and Tanaka is selected;
    - "SS_NT" - the Nakagjima and Tanaka correction factor for RT matrices in SS approximation will be employed;
    - "FT" - flat transmission (ignoring roughness) for transmission matrices will be used.

  If the case of flat surface is chosen, the reflection and transmission will be considered based on Fresnel law's for a mirror reflecting and refracting surface.

- Define depth grid in ocean.
  The depth grid in the ocean can be read from a file or calculated by the program. User can switch between these two options setting in the "Layering of ocean" input line "from file" or "equidistant".

  If "Layering of ocean" is set to "from file", the user must supply a separate file containing the depth grid. The file name should be given in the "Depth grid file name" input line. The file consists of one column and a number of lines containing the depth grid in [m] in ascending order. File has to be started from 0. and finished with the value of the desired bottom depth. At least two values need to be presented.

  If "Layering of ocean" is set to "equidistant", the user needs to define the ocean depth in the "Ocean depth" input line and the desired number of layer in the "Layers number" input line. The corresponding depth grid will be calculated by the program.

- Set pressure, temperature, salinity, density, and chlorophyll concentration profiles.
  The file name containing required information about pressure, temperature, salinity and density profiles as a function of depth in the ocean has to be given by user in the "Profile scenario file name" input line. The input line consists of six entries. The first

entry contains the file name including path. The five additional integer give the column number in the input file corresponding to depth [m], pressure [dbar], temperature [°C], salinity, and density [kg/m^3], respectively.

The file name containing chlorophyll concentration profiles as a function of depth has to be given by user in the "File name for chlorophyll concentration" input line. The input field consists of three entries. The first entry contains the file name including path. Two additional integers give the column number in the input file corresponding to depth [m] and chlorophyll concentration [μg/l] (mg/m^3), respectively.

- Refractive index of water.
  To calculate the Fresnel reflection and transmission matrices one needs to define refractive index of water. Setting in the "Refractive index input type" input line "wl_dep" or "const", the user can perform calculations using the wavelength dependent or constant refraction index, respectively.

  If "Refractive index input type" is set to "const", the user needs to define refractive index of water setting in the "Refractive index of water" input line the real and imaginary part of refractive index. This value will be used for all spectral range.

  If "Refractive index input type" is set to "wl_dep", the user needs to define the file (including path to the directory where this file is located) in the "Refractive index file name" input line.
  Attention:
  - The file containing the refractive index consists of a header and three columns.
  - Each line at the beginning of the file containing any character except of $0, 1, \ldots, 9$, E, e, D, d will be considered as a comment line.
  - First column contains wavelength in ascending order expressed in [μm].
    Second and third columns contain real and imaginary part of the refractive index, respectively.
  - The spectral range where refractive index is given should span actual wavelength range (AWG) chosen for the radiative transfer calculations (see the input parameter "Spectral segment info" in section 3.9)

  To perform calculation of the Fresnel reflection and transmission matrices accounting for the wavelength dependence of the refractive index, the user needs to define the Reference Wavelength Grid (RWG) on which will be calculated matrices. It can be done setting in the "Reference wavelength grid" input line "min", "max" or ""N". The RWG will be defined by the program as follows:

  – "min" - RWG consists of two wavelengths which coincide with minimal and maximal wavelength of the actual wavelength grid (AWG);

  – "max" - RWG contains all actual wavelength within AWG;

  – ""N" - N defines the number of reference wavelength which will be equidistant spaced within AWG.

  The Fresnel reflection and transmission matrices will be calculated at RWG and interpolated at AWG.

- Set absorption coefficients in water.

  General setting:
  The required absorber in water can be selected setting in the "Forward model: marine absorber" input line "t" or "f". The following example illustrates the selection of pure water, chlorophyll, and CDOM based on the chlorophyll concentration as marine absorber:

```
##       Select absorbers in water
## Pure  | Chloro- | CDOM |  CDOM |fulvic| humic |  Other   |
## water | phyll   | -Chl |  -ACR | acid | acid  | absorber |
Forward model: marine absorber
    t        t         t       f      f      f        f
```

  Pure water:
  The absorption coefficient of the pure water as a function of the wavelength should be defined by the user in a separate file. The file name should be given in the "Pure water absorption coefficients file name" input line. The input line consists of three entries. The name of the file containing absorption coefficient should be given as the second entry in this line. User can set the absorption coefficient of the pure water to the desired value setting as the first entry in the same line "f". In this case the third entry in the same line will be considered by program as the required absorption coefficient. The file containing absorption coefficient will be ignored in this case. An example is given as follows:

```
#      File name for absorption coefficient of pure water [m^-1]
Pure water absorption coefficients file name
f  '../../DATA_BASES/SPECTRA_UW/pw_abs_HALTRIN.dat' 0.0257
```

  In the case of such input line the absorption coefficient of the pure water will be set by program to 0.0257 m^{-1} for all wavelengths.
  If the first entry of the "Pure water absorption coefficients file name" is set to "t", the absorption coefficient will be used by program from the file and the third entry will be ignored.
  Note that:
  - the file containing pure water absorption coefficient (it is "pw_abs_HALTRIN.dat" in the example given above) consists of header and two columns. The first column contains wavelength [nm] in the ascending order and the second one the absorption coefficient [m^{-1}].

  Chlorophyll:
  The specific absorption coefficient of chlorophyll as a function of wavelength should be defined by the user in a separate file. The file name should be given in the "Chlorophyll absorption coefficients file name" input line.
  The file containing chlorophyll normalized specific absorption coefficient consists of header and two columns. The first column contains wavelength [nm] in the ascending order and the second one the chlorophyll normalized specific absorption coefficient $A_c(\lambda)$. According to Morel and Maritorena (2001) the chlorophyll related absorption

coefficient (m^{-1}) will be calculated by the program as

$$\alpha_c(\lambda) \;=\; 0.06\, A_c(\lambda)\, C^{\,0.65}\;, \tag{3.23}$$

where $A_c(\lambda)$ is the normalized chlorophyll specific absorption coefficient ($A_c(\lambda_0) = 1$, for the reference wavelength $\lambda_0 = 440\,\mathrm{nm}$), C is the chlorophyll concentration ($\mathrm{mg\,m^{-3}}$). In the current version of SCIATRAN $A_c(\lambda)$ was taken from Prieur and Sathyendranath (1981).

CDOM (Colored Dissolved Organic Matter):
The user can switch between two different approaches to include aborption by CDOM (referred to also as yellow substance) in radiative transfer calculations.

- Setting control parameter "Approximation of CDOM absorption" to "Chl", the approximation of CDOM absorption coefficient related to the concentration of chlorophyll according to model of Morel and Maritorena (2001) will be used. In this case the absorption coefficient $\alpha_\mathrm{p}(\lambda)$ (m^{-1}) was implemented according to Morel and Maritorena (2001) in the following form:

$$\alpha_\mathrm{p}(\lambda) = 0.2\left[\alpha_\mathrm{w}(\lambda_0) + 0.06\, C^{\,0.65}\right] e^{-S(\lambda-\lambda_0)}\;. \tag{3.24}$$

  Here, $\alpha_\mathrm{w}(\lambda_0)$ is the pure water absorption coefficient (m^{-1}) at reference wavelength λ_0, the spectral slope parameter S is set to 0.014 $\mathrm{nm^{-1}}$, parameters C and λ_0 are the same as in Eq. (3.23).
- Setting control parameter "Approximation of CDOM absorption" to "FHa", the approximation of CDOM absorption coefficient related to concentrations and specific absorption coefficients of fulvic and humic acids will be used. In this case the absorption coefficient of CDOM is approximated as a sum of absorption coefficients of fulvic and humic acids as follows:

$$\alpha_\mathrm{p}(\lambda) \;=\; C_f\, a_f(\lambda) + C_h\, a_h(\lambda)\;, \tag{3.25}$$

  where subscript "f" and "h" denotes fulvic and humic acid, respectively, C_f and C_h are concentrations of acids [$\mathrm{g\,m^{-3}}$], $a_f(\lambda)$ and $a_h(\lambda)$ are specific absorption coefficients [$\mathrm{m^2\,g^{-1}}$]. The approximation of specific absorption coefficient $a_f(\lambda)$ and $a_h(\lambda)$ has been implemented according to Carder et al. (1989) in the following form:

$$a_x(\lambda) \;=\; a_x(\lambda_r)\, \exp\left[S_x(\lambda_r - \lambda)\right]\;, \tag{3.26}$$

  where λ_r in [nm] is the reference wavelength, $a_x(\lambda_r)$ is the specific absorption coefficient at this wavelength, and S_x is the spectral slope parameter [$\mathrm{nm^{-1}}$].
  The parameters of specific absorption coefficients can be defined in the "Parameters of specific absorption coefficient" control line which consist of five entries.
  - first entry is the reference wavelength λ_r in [nm];
  - second and third entries are specific absorption coefficient at λ_r and spectral slope for fulvic acid;
  - fourth and fifth entries are specific absorption coefficient at λ_r and spectral slope for humic acid.

An example of this control line is given below.

```
##      Parameterization of fulvic and humic acids specific absorption
##      coefficients to describe CDOM absorption
##      fulvic acid        humic acid
Parameters of specific absorption coefficient
 450.  0.007   0.0194    0.1302   0.011
```

Here, $\lambda_r = 450$, $\alpha_f(\lambda_r) = 0.007$, $S_f = 0.0194$, and $\alpha_h(\lambda_r) = 0.1302$, $S_h = 0.011$.
The concentrations of the fulvic and humic acids can be defined in the separate file using the "Concentrations of fulvic and humic acids" control parameter. The control line consists of two entries

- first entry defines the filename containing concentration of fulvic and humic acids as a function of depth along with the path to the directory where this file is located;
- second entry defines the extrapolation type:
  "Z" - extrapolation with zero values;
  "C" - extrapolation with constant values;
  "L" - linear extrapolation.

The file contaning the concentration of acids consists of the header and three columns:
- first column is the depth in [m];
- second column is concentration of fulvic acid in [$\mathrm{g\,m^{-3}}$];
- third column is concentration of humic acid in [$\mathrm{g\,m^{-3}}$].

All lines at the begining of the file having in the first position symbol `"#", ";", "*" or ">"` will be considered by the program as header lines.

Attention: The control parameter "Approximation of CDOM absorption" has to be set to "FHa" if the fluorescence of CDOM should be accounted for.

Additional absorber in water:
User can introduce any number of additional absorbing components in the water. This can be done using the control parameter "Use additional absorber in water". The first input line of this control parameter consists of three entries:
- the number of absorbers;
- the path to directory containing absorption coefficients;
- the path to directory containing concentration profiles.

If "the number of absorber" does not equal to zero, the following input lines contain information about each additional absorber. Each input line consists of four entries.

- First entry is the file name containing absorption coefficient and corresponding wavelength grid.
  The file consists of header and two columns. Each line at the beginning of file containing in the first position "#", ";", "*", or "¿" will be treated as header line. The first column contains wavelength [nm] in the ascending order and the second one the absorption coefficient [$\mathrm{m^{-1}}$] or absorption cross-section [$\mathrm{m^2/mg}$].
- Second entry is the file name containing concentration of absorber and corresponding depth grid.
  The file consists of header and two columns. Each line at the beginning of file

containing in the first position "#", ";", "*", or "¿" will be treated as header line. The first column contains depth [m] in the ascending order and the second one the concentration of absorber [mg/m^3].

- Third entry is the normalization factor.
  If the absorption coefficient is given in [m^{-1}] than normalization factor is given as a concentration of this species expressed in [mg/m^3] and will be used by the program to calculate the specific absorption coefficient dividing the absorption coefficient by this factor. The actual absorption coefficient will be calculated by the program multiplying obtained specific absorption coefficient by the concentration of absorber.
  If the specific absorption coefficient is given in [m^2/mg], the normalization factor should be set to "1". The actual absorption coefficient will be calculated by the program multiplying this specific absorption coefficient by the concentration of absorber.
- Fourth entry is the type of absorber concentration profile extrapolation.
  It can be set to "C" or "Z".
  "C" - profile will be extrapolated as constant;
  "Z" - extrapolation by zero values.

Wavelength interpolation of absorption coefficients:
User can switch between the Akima and linear interpolation technique. The Akima interpolation technique will be used if in the "Do Akima interpolation" input line one set "t". Otherwise, the linear interpolation will be used.

- Rayleigh scattering in the seawater.
  Setting in the "Pure seawater scattering function" input line "Morel", "Shifrin", "Buiteveld ", the user can switch between three approximate approaches which will be used by program to calculate Rayleigh scattering cross-section in seawater.

  Depolarization ratio can be used as a constant or wavelength dependent.
  The user can switch between these two options setting in the "Pure seawater depolarization ratio" "constant" or "from file" (the last option is not implemented yet in SCIATRAN). If "Pure seawater depolarization ratio" parameter is set to "constant", then the user needs to define the desired depolarization ratio in the "Constant depolarization ratio" input line.

  The optical thickness of the pure seawater can be set by user to any desired value. If the first entry in the "Rayleigh optical thickness of water" input line is set to "t", then the second entry will be interpreted by the program as a desired Rayleigh optical thickness. This option allows, for example, to eliminate impact of different approximations and numerical integration rules comparing SCIATRAN results to benchmark results or other codes.
  Attention:
  - The Rayleigh optical thickness of the seawater is independent of the wavelength if this option is used.

- Scattering and absorption by particulate matter.
  There is two ways to define the scattering properties of the particulate matter in the water. One can use the approximation proposed by Kopelevich or define all needed

parameters in an user-defined file. The desired option can be selected putting in the "Hydrosol angular scattering" input line "Kopelevich" or "User_supplied", respectively. These both options can be used simultaneously if in the "Number of hydrosol models" input line one set "2". In this case the input field in the "Hydrosol angular scattering" input line consists of two subsequent lines. In the first line must be set "Kopelevich" and in the second one "User_supplied". The additional input files, i.e., "kop_hsol.inp" and "man_hsol.inp" should be used, respectively (see description of these input files below). If parameter "Number of hydrosol models" is set to "0" the water will be considered as free of particulate matter (pure water) and setting in "Hydrosol angular scattering" input line will not be used by the program.

- Discretization of scattering matrices.
  The input parameter "Number of streams in ocean" controls the number of Gaussian nodes used to discretize the angular integrals in the radiative transfer equation in ocean. The control line consist of two entry's.
  The first entry (N_1) defines the number of streams in the refraction region (so called Fresnel cone). It should be equal to "Number of streams" as given in "control_ac.inp".
  The second entry (N_2) defines the number of streams in the total reflection range. It should be defined by user.
  The number of Legendre moments retained in the Legendre series expansion of the oceanic scattering phase functions is controlled by the "Number of Legendre moments" input parameter. To estimate the number of streams and Legendre moment one can use the following empirical relationship: 0.43×("Number of Legendre moments" - 1) ≈ $N_1 + N_2$.

- Ocean bottom reflection.
  In the current SCIATRAN version the Lambertian ocean bottom reflection is allowed only. The ocean bottom albedo can be defined in the "Ocean bottom albedo" control line.

- Output of water-leaving radiance.
  Along with the intensity (radiance) of the radiation field the user can obtain as an additional output the water-leaving radiance, i.e., the radiance just above the ocean-atmosphere interface which coming from the water into atmosphere. The output file "water_leaving.dat" is located in the directory "../DATA_OUT" and it has the same format as the standard output file "intensity.dat" (see Section 3.23.1). This output mode will be active if the control parameter "Output of water-leaving radiance" is set to "on".

- Coupling.
  If the control parameter "Coupling" is set to "on", then solution of RTE in the ocean-atmosphere system is obtained iteratively accounting for coupling effects. This means that interactions between atmosphere and ocean is calculated iteratively up to a defined convergence criteria. The second entry value in the "Coupling" control line defines maximal namber of ocean-atmosphere interaction.
  Setting "Coupling" control parameter to "off", the solution of RTE in the ocean-atmosphere system can be obtained ignoring coupling effects. In this case:
  - the discrete-ordinate solution in the atmosphere is obtained under assumption that there is the Fresnel reflection from the ocean surface (no water-leaving radiation

from the ocean);
  - the discrete-ordinate solution in the ocean is obtained under assumption that the ocean-atmosphere interface is illuminated by the direct and diffuse radiation of the atmosphere.
  - the backscattered light from the ocean (ocean leaving radiance) is calculated only once and no response (multiscattered part) of the atmosphere into the ocean is considered in the radiative transfer calculation.

  This option can be used e.g., to estimate errors in the radiative parameters caused by the ignoring of coupling effects in the ocean-atmosphere system.

- Vibrational Raman scattering and fluorescence.
  The radiative transfer within water can be calculated including the vibrational Raman scattering of pure water, fluorescence of chlorophyll-a, and fluorescence of CDOM. The theoretical background and numerous examples are geven in (**?**). To select corresponding inelastic process one should use the "Inelastic processes wihtin water" control parameter. The control line consists of three entries:
  - setting all entries to "off", all inelastic processes will be excluded;
  - setting first entry of this control parameter to "default" or "advanced", the solution of RTE in the ocean-atmosphere system will be obtained accounting for the vibrational Raman scattering process within water;
  - setting second entry to "default" or "advanced", one can include the chlorophyll-a fluorescence;
  - setting third entry to "default" or "advanced", one can include the CDOM fluorescence.

  If the "advanced" option is selected, parameters specific for this mode should be defined by user in the "control_rrs.inp" input file (see below). If the "default" option is selected, the program uses the default values for all needed parameters and no additional setting by user is required.
  An example of this option is given as

```
##  VRS     F_Chl  F_CDOM
Inelastic processes wihtin water
  default    off    off
```

  Limitations:
  - The standard post-processing technique can not be used if VRS and/or fluorescence are included (preliminary restriction). Therefore, if the mode "va" or "ca" is selected (see Section 3.8.1) in the "Angle selection mode" control parameter, the required solution will be obtained employing the linear angular interpolation of the radiation field calculated at a given number of Gaussian nodes.

3.20.1 Input file "kop_hsol.inp"

If the "Hydrosol angular scattering" input parameter in the "control_uwt.inp" file is set to "Kopelevich", then the parameters of hydrosol model have to be defined by user in the file "kop_hsol.inp". SCIATRAN uses in this case the approximation of the angular scattering

coefficient for small and larger particles proposed by Kopelevich (Kopelevich, 1983) (see discussion of this model e.g., by Mobley (Mobley, 1994)). There are the following options:

- Select input form of scattering functions.
  Using "Hydrosol scattering function representation" input line user can switch between two possibilities to import Kopelevich scattering function into SCIATRAN:
  - "Expansion_coeff" - the scattering function is represented by the Legendre series expansion coefficients. The filenames containing the expansion coefficients should be specified for the small and larger particles in the "File names containing expansion coefficients" input line. The path to the directory containing corresponding files should be given in "Directory name for scattering matrices" input line. The input field consists of two entries:
    first entry - filename for small particles;
    second entry - filename for larger particles.
  - "Scattering_matrix" - the scattering functions for small and larger particles are given as a function of the scattering angle. The filenames containing scattering functions should be specified in the "File names containing scattering function/matrix" input line. The path to the directory containing corresponding files should be given in "Directory name for scattering matrices" input line.
- Define concentration profiles of small and larger particles.
  The input fields in "Particulate matter concentration" input line should be used to define concentration of the small and large particles as a function of the depth. Input field format for this option is given by the following example:

```
Particulate matter concentration
3
 0.0   0.1  0.03
10.0   0.1  0.03
20.0   0.1  0.03
```

  The first input line contains the number of input levels where the concentration will be given (3 in this cse). Subsequent lines (number of subsequent lines equal to number of input levels) consist of three columns: first column is the depth in [m] in ascending order; second and third columns contain the relative concentration of the small and larger particles, respectively.
  Attention:
  - minimum two depth levels are required;
  - the vertical profiles of small and larger particles will be linearly interpolated between the input altitude levels and extrapolated with zero above the highest and below the lowest input level.
  - concentration of small and larger particles have to be given in [ppm] or [cm^3/m^3].

  Note that
  - the small fraction represents terrigenous particles with density $\rho_s = 2$ g cm^{-3}, relative (to the water) refractive index $n_s = 1.15$, and the size distribution in the region [0.01,1.3] μm;
  - the larger fraction represents organic particles of phytoplankton and detritus with the density of $\rho_l = 1$ g cm^{-3}, relative refractive index $n_s = 1.03$, and the size

distribution in the region [1.3,13] μm.

3.20.2 Input file "man_hsol.inp"

If the "Hydrosol angular scattering" input parameter in the "control_uwt.inp" file is set to "User_supplied", then the parameters of hydrosol model have to be defined by user in the file "man_hsol.inp". There are the following options:

- Number of hydrosol layers and their bottom depths.
  The number of hydrosol layers is given in "Layering of scattering function/matrix" input line. The subsequent line contains bottom depths [m] (in the ascending order) of all hydrosol layers.
  Attention:
  - only single scattering phase function can be defined within each hydrosol layer (see below).

- Select reference wavelengths.
  To take into account the spectral dependence of scattering functions/matrices, as well as scattering and extinction coefficients the hydrosol optical characteristics can be defined by user at the number of reference wavelengths. The number of wavelengths is given in "Number of wavelength and wavelength grid" input line. In the subsequent line the wavelength grid [nm] in the ascending order should be given.
  Attention:
  - at least two reference wavelengths are required;
  - the output wavelength grid (see Section 3.9) should be within reference wavelengths where the hydrosol optical characteristics are given.

- Select input form of scattering functions/matricies.
  Using "Hydrosol scattering function representation" input line user can switch between three possibilities to import hydrosol scattering function into SCIATRAN:

  – "Asymmetry_factor" - the hydrosol scattering function is defined by the asymmetry factor according to the Henyey-Greenstein parameterization. The asymmetry factor should be specified for each hydrosol layer and all reference wavelengths in "Asymmetry factor values" input line. The input field format is given by Eq. (3.27)

$$\begin{matrix} P_{1,1} & P_{1,2} & \dots & P_{1,N_\lambda} \\ P_{2,1} & P_{2,2} & \dots & P_{2,N_\lambda} \\ \dots & \dots & \dots & \dots \\ P_{L,1} & P_{L,2} & \dots & P_{L,N_\lambda} \end{matrix} \tag{3.27}$$

  where $P_{i,k}$ is the asymmetry factor in the hydrosol layer i and reference wavelength k.

  – "Expansion_coeff" - the hydrosol scattering function is represented by the Legendre series expansion coefficients. The filenames containing the expansion coefficients should be specified for each hydrosol layer and reference wavelength in the "File

names containing expansion coefficients" input line. The path to the directory containing corresponding files should be given in "Directory name for scattering matrices" input line. The input field format is given by Eq. (3.28) where $P_{i,k}$ is the file name containing expansion coefficients in the aerosol layer i and reference wavelength k. The file containing expansion coefficients is formatted as follows:

```
Example of the file containing expansion coefficients
Numerical accuracy = 0.10D-06
CEXT   = 0.339753D+01; CSCA  = 0.339753D+01
ALBEDO = 0.10D+01;     <COS> = 0.783276D+00
  S   Alpha 1
>
  0   1.00000
  1   2.34983
  2   3.45081
  3   3.78591
  4   4.30796
  5   4.54277
  6   4.88813
```

In this example first 6 lines will be considered as comment lines. In fact the number of comment lines in the file header is arbitrary. Each line containing any character except of $0, 1, \ldots, 9$, E, e, D, d will be considered as a comment line. The first column in the data block (after line beginning with >) has to be presented but is not used. The number of lines in the data block corresponds to the number of moments needed for the appropriate representation of scattering function (only seven lines is shown in the example above). The subsequent data block contains the expansion coefficients in the second column.
Attention:

- The reading of moments (lines) in this file will be finished if
  - end-of-file is reached;
  - expansion coefficient in a line is zero;
  - the number of read moments greater than 5000.

– "Scattering_matrix" - the hydrosol scattering function is given as a function of the scattering angle. The filenames containing scattering functions should be specified for each hydrosol layer and reference wavelength in the "File names containing scattering function/matrix" input line. The path to the directory containing corresponding files should be given in "Directory name for scattering matrices" input line. The input field format is given by Eq. (3.28) where $P_{i,k}$ is the file name containing scattering matrix in the aerosol layer i and reference wavelength k.
Limitation:

- this option is not allowed in the vector case.

Input field format for these three option is given in the control file "man_hsol.inp" by

$$\begin{array}{cccc} P_{1,1} & P_{1,2} & \dots & P_{1,N_\lambda} \\ P_{2,1} & P_{2,2} & \dots & P_{2,N_\lambda} \\ \dots & \dots & \dots & \dots \\ P_{L,1} & P_{L,2} & \dots & P_{L,N_\lambda} \end{array} \tag{3.28}$$

where L is the number of hydrosol layers and N_λ is the number of reference wavelengths.

The parameterization has to be supplied in a file which is formatted as follows. The subsequent data block contain scattering angles in degrees in the first column and appropriate values of the phase function in the second column.

- Define extinction coefficient and single scattering albedo vertical profiles.
  In contrast to the scattering function the extinction coefficient and single scattering albedo (SSA) can be defined as a function of depth even if only single hydrosol layer is selected. The input fields in "Extinction coefficient" and "Single scattering albedo" input lines should be used to introduce these vertical profiles. Input field format for these two option is given by

$$\begin{array}{ccccc} N_z & & & & \\ Z_1 & P_{1,1} & P_{1,2} & \dots & P_{1,N_\lambda} \\ Z_2 & P_{2,1} & P_{2,2} & \dots & P_{2,N_\lambda} \\ \dots & \dots & \dots & \dots & \dots \\ Z_{N_z} & P_{N_z,1} & P_{N_z,2} & \dots & P_{N_z,N_\lambda} \end{array} \tag{3.29}$$

  where $P_{j,k}$ is extinction coefficient (expressed in $[\mathrm{m}^{-1}]$) or SSA, respectively, at the depth Z_j and k-th wavelength. N_z is the number of depths, Z_j is the depths [m], and N_λ is the number of reference wavelengths.
  Attention:
  - minimum two depth levels are required, i.e., $N_z \geq 2$;
  - the vertical profiles of extinction coefficients and SSA will be linearly interpolated between the input altitude levels and extrapolated with zero above the highest and below the lowest input level.

3.20.3 Vibrational Raman scattering in ocean

Appropriate control files: "control.inp", "control_uwt.inp", "control_rrs.inp"
Relevant control parameters: "Add TRS to extinction", "Basic spectroscopic parameters", "Depolarization ratio" "Exclude solar light", "Integrate with FRF", "Numerical technique used for VRS", "Total Raman scattering coefficients"

Setting the "Include radiative transfer within ocean or ice" control parameter in the control file "control.inp" to "ocean" and the first entry of the "Inelastic processes wihtin water" control parameter in the control file "control_uwt.inp" to "default" or "advanced", radiative transfer calculations within ocean will be performed accounting for the vibrational Raman scattering of H_2O molecules in water.

If the first entry of the "Inelastic processes wihtin water" control parameter is set to "default" then default setup of all needed parameters to account for vibrational Raman scattering will be used automatically by the program (no action from user is needed). Default values are shown below using this color.
If the first entry of the "Inelastic processes wihtin water" control parameter is set to "advanced" then parameters specific for this mode should be selected by user in the "control_rrs.inp" input file as follows:

- Two different techniques can be selected by user to solve RTE including VRS:
  - setting "Numerical technique used for VRS" control parameter to "dom" the standard discrete-ordinates technique will be used;
  - setting this control parameter to "adj" the forward-adjoint approach will be employed.
    Attention: This mode is not properly validated yet and it is not recommended for usage.

  Default value is "dom".

- Setting the first entry in "Total Raman scattering coefficients" control parameter to "t", the user-defined total Raman scattering coefficients at excitation and emission wavelengths will be used by the program as second and third entry values in this control line.
  Default value is "f".
  These parameters will be considered as total Raman scattering coefficient [m^{-1}] at excitation and emission wavelength wavelength, respectively.
  Attention:
  Total Raman scattering coefficients are the same for all required excitation and emission wavelengths. This option is recommended to use only for test purpose and for the comparison with results obtained with other RTM with the predefined total Raman scattering coefficients.

  If the first entry of the "Total Raman scattering coefficients" control parameter is set to "f", the second and third entries should be present but they will not be used by the program. The wavelength dependence of the total Raman scattering coefficient will be defined in the "Basic spectroscopic parameters" control parameter (see below).

- The depolarization ratio of the vibrational Raman scattering of water molecules should be defined in the "Depolarization ratio" control parameter.
  Default value is "0.17".

- The basic spectroscopic parameters needed for computation of radiative transfer including vibrational Raman scattering within water should be defined using "Basic spectroscopic parameters" control parameter consisting of five entries:

  – first entry defines how the second entry parameter will be considered by the program:
    - if the first entry is set to "TRS" than the second entry will be considered by the program as the total Raman scattering coefficient;
    - if the first entry is set to "CS_90" than the second entry will be considered by the program as the Raman scattering cross section at the scattering angle

equal to 90°.

- second entry presents the value of either TRS [m^{-1}] or cross section [cm^2/(molecule sr)] (as specified by the first entry);
- third entry specifies the reference wavelength [nm] where TRS or CS_90 is given;
- fourth entry specifies wavelength dependence of the total Raman scattering coefficient and can be set to "Resonance" or to "Inverse power law", which given, respectively, by following expressions:

$$\beta_{\rm vrs}(\nu') \;=\; \beta_0^R\,\frac{1}{N_r}\,\frac{\nu^4}{(\nu_i^2-\nu'^{\,2})^2}\;,\quad \beta_{\rm vrs}(\nu') \;=\; \beta_0^R\left(\frac{\nu'}{\nu_r}\right)^n\;, \tag{3.30}$$

where $\beta_{\rm vrs}(\nu')$ and β_0^R are total Raman scattering coefficients at the excitation wavenumber ν' and reference wavenumber ν_r, respectively, $\nu = \nu' - \Delta\nu$ is the emission wavelength and $\Delta\nu$ is the Raman shift (~ 3400 cm^{-1}). ν_i is the relevant intermediate energy level for water, N_r is the normalization factor given by

$$N_r \;=\; \frac{(\nu_i^2-\nu_r'^{\,2})^2}{\nu_r^4}\;,\quad \nu_r' \;=\; \nu_r \;+\; \Delta\nu\;. \tag{3.31}$$

- fifth entry
  defines position of the intermediate energy level ν_i for water [nm] if "Resonance" is selected;
  defines the value of exponent n if the fourth input parameter is set to "Inverse power law".

Default values are

```
Basic spectroscopic parameters
      TRS    2.7d-04    488.   'Resonance'    130.
```

- If the first entry of "Add TRS to extinction" control parameter is set to "t", then the total vibrational Raman scattering coefficient will be added to the absorption coefficient of pure water at all excitation wavelengths.
  If the second entry of "Add TRS to extinction" control parameter is set to "t", then the total vibrational Raman scattering coefficient will be added to the absorption coefficient of pure water at all emission wavelengths to describe properly the energy loss due to trans-spectral Raman scattering.
  This control parameter should be set to "f f" if absorption coefficients of water includes already the contribution of Ramn scattering.
  Default value is "f t".

- The user can switch between two possibilities to calculate contribution of the Raman scattering into intensity at a required emission wavelength. Fig. 3.1 shows a frequency redistribution function (FRF) corresponding to 488 nm emission line. Setting the first entry of the "Integrate with FRF" control parameter to "t" one forces the program to integrate Raman scattering contribution with FRF over a required spectral range around excitation wavelength (area under solid line in Fig. 3.1). If this option is chosen, the second entry will be considered by program as wing cut-off (HWHM number of

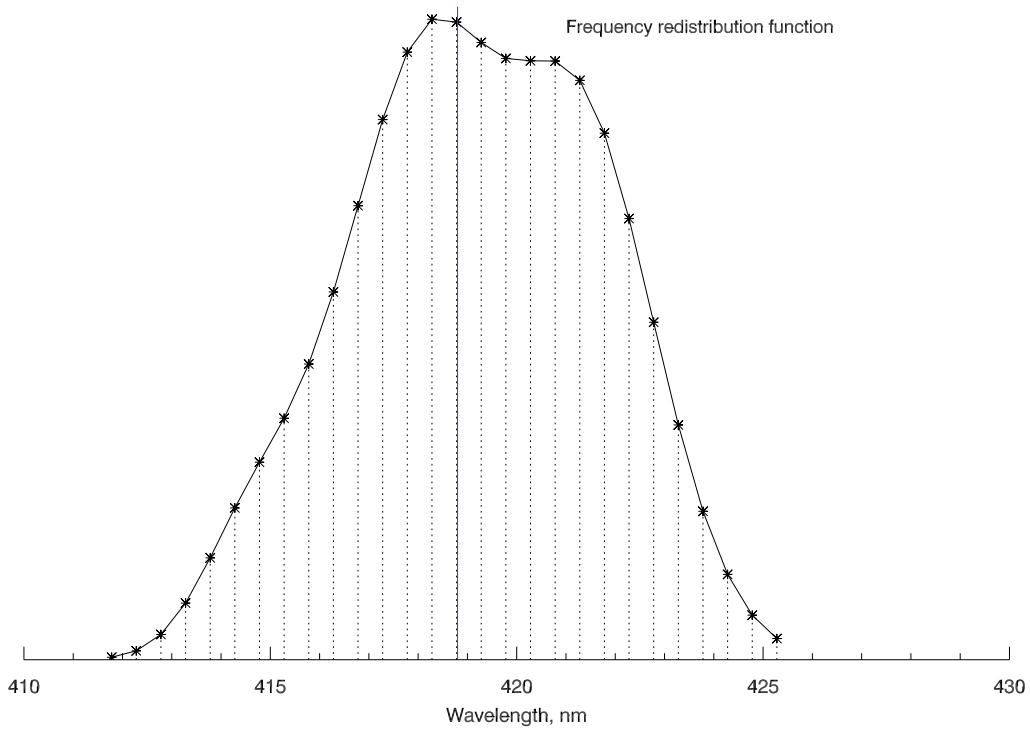

Figure 3.1: Frequency redistribution function for 488 nm emission wavelength.

FRF) and the third one gives integration wavelength step [nm] (distance between two adjustment vertical doted lines in Fig. 3.1).
If the first entry is set to "f" two following entries will be ignored by the program and only single excitation wavelength corresponding to the maximum of FRF will be used (position of this wavelength is shown in Fig. 3.1 by the vertical red solid line).
Attention:
This option is significantly quickly but less accurately as compare to the integration with FRF.
Default values are

```
Integrate with FRF
t  2.0  0.5
```

- Setting the "Exclude solar light" control parameter to "t", the calculation of radiative transfer at an emission wavelength will be performed without contribution of the solar light at this wavelength, i.e., the radiative transfer of the inelastically scattered radiation only will be considered at the emission wavelength.
  Attention:
  This is very specific option. Use it only if you really understand what it means!
  Default value is "f".

3.20.4 Chlorophyll-a fluorescence in ocean

Appropriate control files: "control.inp", "control_uwt.inp", "control_rrs.inp"
Relevant control parameters: "Numerical technique used for fluorescence", "Integration step over Chl excitation range", "Quantum efficiency", "Gaussian emission band parameters"

Setting the "Include radiative transfer within ocean or ice" control parameter in the control file "control.inp" to "ocean" and the second entry of the "Inelastic processes wihtin water" control parameter in the control file "control_uwt.inp" to "default" or "advanced", radiative transfer calculations within ocean will be performed accounting for Chlorophyll-a fluorescence in water.
If the second entry of the "Inelastic processes wihtin water" control parameter is set to "default" then default setup of all needed parameters to account for Chlorophyll-a fluorescence will be used automatically by the program (no action from user is needed).
Default values are shown below using this color.
If the second entry of the "Inelastic processes wihtin water" control parameter is set to "advanced" then parameters specific for this mode should be selected by user in the "control_rrs.inp" input file as follows:

- Two different techniques can be selected by user to solve RTE including Chl-a fluorescence:
  - setting "Numerical technique used for fluorescence" control parameter to "dom" the standard discrete-ordinates technique will be used;
  - setting this control parameter to "adj" the forward-adjoint approach will be employed.
    Attention: This mode is not implemented yet.

  Default value is "dom".

- The integration over the excitation spectral range (370 - 690 nm) will be performed automatically by the program. The user should select the integration step in "Integration step over Chl excitation range" control parameter. The first entry will be considered by the program as integration step in [nm].
  Default value is "1.".

- Quantum efficiency of this emission process should be defined in "Quantum efficiency" control parameter.
  Default value is "0.01".

- Parameters of the Chl-a fluorescence Gaussian emission band should be defined in "Gaussian emission band parameters" control parameter. First entry defines position of maximum in [nm], second entry is standard deviation [nm].
  Default values are "685. 10.6".

3.21 Parallel execution

Appropriate control files: "control.inp"
Relevant control parameters: "Parallel wavelength loop"

The control parameter "Parallel wavelength loop" can be used to perform parallel calculations on multi processor computer systems using the Open MP standard. At present, Open MP compiler options are employed only on IBM Regatta computers, whereas for other computer systems appropriate adjustment of compiler flags in "Makefile" are necessary. Is is not recommended to make parallel computations on 2 CPU systems. Setting "Parallel wavelength loop" parameter to "t" automatically reduce the screen output.
Limitation:

- at present, parallel calculations can only be performed in the "CDI" mode (see Section 3.6).

3.22 Control output

3.22.1 Standard output

Appropriate control files: "control.inp".
Relevant control parameters: "Screen output", "Output format specification".

Automatically generated by the program output files:
"SCE_ABSORBER.OUT", "SCE_ABSORBER-WATER.OUT", "SCE_AEROSOL.OUT", "SCE_CLOUD.OUT", "SCE_INP-PARS.OUT", "SCE_KOP-HSOL.OUT", "SCE_MAN-HSOL.OUT", "SCE_RAYLEIGH.OUT", "SCE_SUMMARY.OUT", "SCE_VHL.OUT", "errors.log".

- Level of details in the screen output.
  The level of details in the screen output is controlled by the "Screen output" input parameter. Using this flag the screen output of the program or the output to auxiliary files is controlled. The control field requires three string parameters. The first parameter can be set to either "S" or "F" directing the output to the screen (default mode) or to the logfile (LogFile.out) respectively. The second and third parameters control the level of details in the screen output from the radiative transfer model and retrieval block, respectively. The following entries are supported:
  - "N" - no screen output is performed with exception of the final status message.
  - "R" - reduced screen output, only the essential information is written out.
  - "S" - standard screen output, more detailed screen output with intermediate messages.
  - "E" - extended screen output, a lot of details concerning the program progress are written out.
  - "D" - debugging mode, all available program messages are written out. This mode is only useful for debugging purposes.

  Both the second and third parameters might contain "T" as the second character in the string, e.g., "ST", which resuults in running the program in the tracing mode, i.e., the sequence of called by the program routines will be written out.

- Additional output files generated automatically.
  Additionally to the screen output, most important settings used for the radiative transfer modeling and for the retrieval (if appropriate) are stored in the

"SCE_INP-PARS.OUT" and "SCE_SUMMARY.OUT" files, whereas the "SCE_ABSORBER.OUT", "SCE_RAYLEIGH.OUT", "SCE_AEROSOL.OUT", and "SCE_CLOUD.OUT" files contains a short summary of the employed gaseous absorber, Rayleigh, aerosol, and cloud settings, respectively.
If the radiative transfer in the ocean was considered also the "SCE_ABSORBER-WATER.OUT", "SCE_RAYLEIGH.OUT", "SCE_KOP-HSOL.OUT" and "SCE_MAN-HSOL.OUT" files contains a short summary of the employed water absorber, Rayleigh water, and hydrosol settings. These files are located in the subdirectory "./DATA_OUT/".
Attention:

- if the "RTM_TYPE" control parameter is set to "vhl" (vertically homogeneous layer) in "control.inp" file, then "SCE_VHL.OUT" output file will be generated by the program, whereas files "SCE_ABSORBER.OUT", "SCE_RAYLEIGH.OUT", "SCE_AEROSOL.OUT" will not be present;
- files "SCE_KOP-HSOL.OUT" and "SCE_MAN-HSOL.OUT" can not be generated by the program if scattering by hydrosol particles was not taken into account.

The file "errors.log" located in the main program directory contains error and warning messages generated by the program. If "errors.log" file is not empty, i.e., any messages were generated during the last program run, it will be indicated at the end of the screen output, even if the "Screen output" parameter is set to "N", by one of the following messages:

- `********** See errors.log for WARNINGS **********`
- `SCIATRAN stopped in spher_rad: see errors.log`
- `SCIATRAN stopped in dom_spherical: see errors.log`
- `SCIATRAN stopped in gt_iface: see errors.log`

3.22.2 Extended output

Appropriate control files: "control_out.inp"
Relevant control parameters:
"Fluxes for path representation",
"Intensity or Stokes vector output format",
"Intensity representation in output file",
"Lower and upper boundary of flux results",
"Output of following Stokes components",
"Output of surface albedo",
"Output format for multiple wavelengths",
"Output of ellipsometric parameters",
"Put AOT into output file",
"Transform to reflection function?",
"Write local optical parameters"

The extended SCIATRAN output can be used if the "Output format specification" parameter in the "control.inp" file is set to "t". In the "control_out.inp" file the user can specify layout, output formats and desired transformation of the calculated intensity and Stokes vector. There are the following options:

- Select number of output Stokes components.
  The number of Stokes vector components to be printed out (from 1 to 4) can be defined in the "Output of following Stokes components" input line. The input field consists of two entries. The entries define numbers of the Stokes vector component which will be put in the output file. For example, in the case of the following input line:
  `Output of following Stokes components`
  `1 3`
  output file contains first, second, and third Stokes vector components.
  Default setting: "1 4".

- Output of ellipsometric parameters.
  The program can generate the separate file "./DATA_OUT/ellipse_par.dat" containing so-called ellipsometric parameters, i.e.,

  – degree of polarization :

$$DP \;=\; \frac{\sqrt{Q^2+U^2+V^2}}{I}\;, \tag{3.32}$$

  – degree of linear polarization,

$$DLP \;=\; \frac{\sqrt{Q^2+U^2}}{I}\;, \tag{3.33}$$

  – degree of circular polarization,

$$DCP \;=\; \frac{V}{I}\;, \tag{3.34}$$

  – ellipticity,

$$\beta \;=\; \frac{1}{2}\,\arctan\left[\frac{V}{\sqrt{Q^2+U^2}}\right]\;,\;\; |\beta| \le \pi/4\;, \tag{3.35}$$

  – direction the plane of polarization.

$$\chi \;=\; \frac{1}{2}\,\arctan\left[\frac{U}{Q}\right]\;,\;\; \mathrm{sgn}\{\cos 2\chi\} \;=\; \mathrm{sgn}\{Q\}\;,\;\; Q \;\neq\; 0\;, \tag{3.36}$$

$$\chi \;=\; \pi/4\;,\;\; Q \;=\; 0\;,\;\; U \;>\; 0\;, \tag{3.37}$$

$$\chi \;=\; 3\pi/4\;,\;\; Q \;=\; 0\;,\;\; U \;<\; 0\;, \tag{3.38}$$

  where "sgn" means "sign of". We note that in the case of unpolarized light $Q = U = V = 0$ or circular polarization $Q = U = 0$ the polarization angle χ is undefined and will be set to "-999" in the output file.
  Attention:

  * Polarization angle χ given by Eqs. (3.37) - (3.38) corresponding to $Q = 0$ will be selected for all $|Q| \le 1 \cdot 10^{-12}$ otherwise Eq. (3.36) will be used.

This file will be generated by the program if the control parameter "Output of ellipsometric parameters" is set to "yes".
Default setting: "no".

- Output of fluxes at the bottom and top of the atmosphere.
Setting the "Fluxes for path representation" input parameter to "yes" forces the program to output total fluxes at the bottom, $T_d(\vartheta_0)$, and at the top of atmosphere, $T_u(\vartheta_v)$, calculated under assumption of illumination from above and illumination from below, respectively. These fluxes are often used in the following representation of TOA reflectance:

$$R(\vartheta_v, \varphi_v, \vartheta_0) \;=\; R_0(\vartheta_v, \varphi_v, \vartheta_0) \;+\; \frac{T_d(\vartheta_0) T_u(\vartheta_v) A}{1 - sA}\,, \tag{3.39}$$

where $R_0(\vartheta_v, \varphi_v, \vartheta_0)$ is the reflectance of the atmosphere with a black underlying surface, s is the spherical albedo, and A is the Lambertian surface albedo.
Results are in "./DATA_OUT/Trans_Dn.dat" and "./DATA_OUT/Trans_Up.dat" files.
Default setting: "no".
Attention:
  - to use this option the "RTM Mode" control parameter should be set to "wf" (see Section 3.1.6).

- Output of the Lambertian surface albedo.
Setting the "Output of surface albedo" input parameter to "yes" forces the program to output of surface albedo at all wavelengths (result in "./DATA_OUT/albedo_wl.dat").
Default setting: "no".

- Output in the form of the reflection function.
If the transformation of the reflected intensity to the dimensionless reflection function is needed, then the user must set the "Transform to reflection function?" input line to "t".
Default setting: "f".

- Output altitude range of fluxes and spherical albedo in the atmosphere.
User can define the output altitude range for fluxes and spherical albedo in output files. Lower and upper boundary in [km] has to be given in the "Lower and upper boundary of flux results" input line.
Default setting: "0" "120".

- Output of aerosol optical thickness.
The aerosol optical thickness can be put as the output parameter in the "intensity.dat" output file. To use this option the user must set in the "Put AOT into output file" input line "t".
Attention:
  - all other output layouts for the intensity/Stokes vector (see below) will be ignored;
  - output layout in the "Output format for multiple wavelengths" will be set automatically to "wl_in_line" (see below).

  Default setting: "f".

- Output of all local optical parameters.
The following local optical parameters can be written out:

- gaseuos absorption ("gas_abs.dat")
- Rayleigh scattering ("ray_sca.dat")
- aerosol scattering and absorption ("aer_sca.dat", "aer_abs.dat")
- scattering and absorption of clouds ("cld_sca.dat", "cld_abs.dat")

if the first entry in control parameter "Write local optical parameters" is set to "t". The local optical parameters are written out at all altitude levels and all wavelengths. The second control parameter in control line "Write local optical parameters" can be set to "opt_th" or "as_c" specifying whether output files contain optical thicknesses or absorption/scattering coefficients, respectively. The third entry specifies the otput directory.

- Select output layout of intensity/Stokes vector.
  If parameter "Put AOT into output file" is set to "f" the arrangement of the intensity/Stokes vector values in the output file "./DATA_OUT/intensity.dat" can be changed by user if "Angle selection mode" set to "all" (see "control_geom.inp").
  The possible layout of the intensity/Stokes vector depends on the number of wavelength used:
  - The layout for a single wavelength:
    A desired layout in this case can be specified in the "Intensity representation in output file" control line in the form of `"|XXX\YYY|"`, where `"XXX"` defines the name of the angular variable changing with the row number (i.e., vertical) and `"YYY"` defines the name of the variable changing with the column number (i.e., horizontal). For example, `"|Zen\Azm|"` means that the row index is running over zenith angles and the column index over the azimuth angles, i.e., each output line contains intensity values at one zenith angle and all azimuthal angles.
    The following layouts are available:
    ```
    Single solar zenith angle: "|Zen\Azm|" or "|Azm\Zen|"
    Single zenith angle      : "|SZA\Azm|" or "|Azm\SZA|"
    Single azimuthal angle   : "|SZA\Zen|" or "|Zen\SZA|"
    ```
    Additionally the "dynamic" setting can be used which extents vertically the longer array, i.e., the angular variable with larger number of required elements will be changing with the row number.
  - The layout for multiple wavelength:
    The layout in this case can be select in the "Output format for multiple wavelengths" input line. The possible choice is as follows:
    "wl_in_colm" - the values of the intensity/Stokes vector at all line of sights are written out in one line for each particular wavelength. The wavelengths change with the row index. This is the DEFAULT output mode in SCIATRAN.
    "wl_in_line" - the values of the intensity/Stokes vector at all wavelengths are written out in one line for each particular line of sight. The lines of sight change with the row index.

  Default setting: "wl_in_colm".

- Output format for the intensity/Stokes vector.
  The output format can be selected by the user in the "Intensity or Stokes vector output format" input line. This control line can be used to change manually the output format for the intensity/Stokes vector. In the "Intensity or Stokes vector output for-

mat" a valid FORTRAN format string can be supplied to format the output, e.g., "'(1X,F12.7,*(2X,E15.7))'".
Default setting: "default".
Attention:

- Use this format specification if you know what you are doing! Otherwise use "default" format specification setting in the "Intensity or Stokes vector output format" input line "default". The user is responsible for the usage of the correct FORTRAN syntax. Wrong syntax will result in the run time error during the output, all calculation results will be lost!

3.23 Output files

All data files described in this section are located in "./DATA_OUT/" subdirectory of main program directory. At each program run the "output_map.inf" file is generated containing the following information:

- The first line of the header contains the software version followed by the radiative transfer solver (see Section 3.6) and the sphericity mode (see Section 3.4) in brackets, i.e., "DOM, spherical mode, scalar RT" means that the Discrete Ordinate solver was used for the spherical atmosphere without polarization:
  ```
  #  SCIATRAN 3.8.4 (DOM, spherical mode, scalar RT)
  ```
- Subsequent lines in the header contain the name of products generated in the last program run and corresponding filenames, for example:
  ```
  #  Radiance: intensity.dat
  #  Weighting functions:  wf_o3.dat wf_temp.dat wf_press.dat wf_albedo.dat
  #  Stokes components (SC): I-1; Q-2; U-3; V-4
  ```
  Please note, only files listed here were generated during the last program run. Any other files potentially located in "./DATA_OUT/" must not be considered as results.
- The last line in the header contain a legend to the data below, for example:
  ```
  #  Number, SC,   SZA,   LOS angle, azimuth angle(@ TOA); output altitude
  ```
- The lines below the header contain the following information for each output point or direction (so-called measurement coordinates):
  - output point (or direction) number;
  - component of the Stokes vector;
  - local solar zenith angle at the output point;
  - line-of-sight viewing angle and azimuth angle (if necessary);
  - altitude of the output point.

  Example of the full output:
  ```
  #  SCIATRAN 3.8.5 (DOM, plane-parallel mode, scalar RT)
  #  Radiance: intensity.dat
  #  Weighting functions:  wf_no2.dat
  #  Stokes components (SC): I-1; Q-2; U-3; V-4
  #  Number, SC,   SZA,   LOS angle, azimuth angle(@ TOA); output altitude
     1       1    70.00    10.00       30.41     100.00
     2       1    75.00    10.00       30.41     100.00
     3       1    80.05    10.00       30.41     100.00
  ```

Dependent on the RTM mode selected in the "RTM Mode" control line (see Section 3.1) different output files will be generated. The names and formats of output files generated in different program modes are discussed below in details. Similar to the "output_map.inf" file, the first header line in each output file contains the software version followed by the radiative transfer solver and the sphericity mode in brackets.

Beside the main output files described in this section, a set of temporary output files can be written out during a program run. These files are intended for control and debugging purposes and are irrelevant for an ordinary user.

3.23.1 Intensity/Stokes vector ("RTM Mode" is set to "int")

The calculated intensity/radiance and components of Stokes vector are stored in "intensity.dat" file. The structure of the files "output_map.inf" and "intensity.dat" depends on the control parameters "Intensity representation in output file" and "Output format for multiple wavelengths" as well as on the number of solar and viewing angles, and the number of wavelengths. We consider at first a most general case of multiple angles and multiples wavelengths.

Let as assume that the intensity of radiation field should be calculated at TOA, at the solar zenith angles 50° and 70°, viewing zenith angles 15° and 25°, azimuthal angles 30° and 90°, and at the wavelengths 500 and 550 nm.
An example of the "output_map.inf" file is given in this case as follows:

```
#  SCIATRAN 3.8.4 (DOM, plane-parallel mode, scalar RT)
#  Radiance: intensity.dat
# Geometry data: each line of this file lists angles for each column
#                in intensity.dat  file
# 1st column : sequential number of the line of sight
# 2nd column : number of the Stokes component
# 3rd column : solar zenith angle at the output altitude in degrees
# 4th column : viewing angle at the output altitude in degrees
# 5th column : relative azimuth angle at the output altitude in degrees
# 6th column : geometrical tangent height in km (999 if TH is not in
#              the viewing direction)
# 7th column : refractive tangent height in km (999 if TH is not in
#              the viewing direction)
# 8th column : solar zenith angle (refractive) at the tangent height
#              or at the end of the line of sight(if TH is not in the
#              viewing direction) in degrees
#              (set to 180 if the point is not illuminated)
# 9th column: single scattering angle (refractive) at the tangent
#             height or at the end of the line for downward pointing
#             LOS or at the first point for upward pointing LOS
#             (set to 90 if the point is not illuminated)
# 10th column: ouput altititude in km
  1  1   50.00   15.00   30.00  999.00  999.00   50.00  116.67   60.00
  2  1   50.00   15.00   90.00  999.00  999.00   50.00  128.38   60.00
  3  1   50.00   25.00   30.00  999.00  999.00   50.00  107.61   60.00
  4  1   50.00   25.00   90.00  999.00  999.00   50.00  125.63   60.00
  5  1   70.00   15.00   30.00  999.00  999.00   70.00   96.85   60.00
  6  1   70.00   15.00   90.00  999.00  999.00   70.00  109.29   60.00
  7  1   70.00   25.00   30.00  999.00  999.00   70.00   88.07   60.00
```

```
 8  1   70.00   25.00   90.00  999.00  999.00   70.00  108.06   60.00
```

The first line of the header contains the software version followed by the radiative transfer solver (see Section 3.6) and the sphericity mode (see Section 3.4) in brackets, i.e., "DOM, plane-parallel mode, scalar RT" means that the Discrete Ordinate solver was used for the plane-parallel atmosphere without polarization.
The second line in the header contains the name of products generated in the last program run and corresponding filenames.
The third line contains the information for user that "each line of this file lists angles for each column in intensity.dat file".
Other lines in the "output_map.inf" file explain content of columns in the data block.
The "intensity.dat" file containing results of calculation is given by

```
#  SCIATRAN 3.8.4 (DOM, plane-parallel mode, scalar RT)
#  Contents: Wavelength [nm], Radiance [phot/s/cm^2/nm/sr]
#  Irradiance: Pi (3.1415926536) [phot/s/cm^2/nm]
 500. 1.940E-01 1.979E-01 1.928E-01 1.983E-01 1.036E-01 1.054E-01 1.047E-01 1.065E-01
 550. 1.782E-01 1.808E-01 1.769E-01 1.806E-01 9.107E-02 9.226E-02 9.151E-02 9.276E-02
```

- The first line in this file contains the same information as first line in the "output_map.inf" file.
- The second line of the header contains the product name, i.e., "Radiance", followed by the output units: "phot/s/cm^2/nm/sr".
- The first data column contains the wavelength information and all other columns contain the radiances appropriate to different output points or directions. The output sequence is the same for both radiances and measurement coordinates in "output_map.inf", i.e., the radiance contained, for example, in the third data column (i.e., for the second line-of-sight) is appropriate to the output point and direction defined by the measurement coordinates in the second data line in the "output_map.inf" file, i.e, $\{\vartheta_0, \vartheta, \varphi\} = \{50°, 15°, 90°\}$

3.23.2 Weighting functions ("RTM Mode" is set to "wf")

Intensity/radiance is stored in "intensity.dat" file as described in Section 3.23.1. Weighting function for the selected parameters (see Section 3.1.6) are stored in separate files named "wf_{parameter name}.dat", where "{parameter name}" can be, for example, "o3", "press", "albedo" and so on. Exact names of the weighting function files generated by the program according to the selected parameters are listed in the header of the "output_map.inf" file. All weighting function files have the same format:

- The second line of the header contains the product name, i.e., "Weighting functions", followed by the output units: "sun normalized" if "Extra-terrestrial solar flux" control parameter was set to "Pi" or "Unity" or "photons/s/nm/cm2/ster"
  if "Extra-terrestrial solar flux" was set to "File" (see Section 3.2), except for average number of photon scattering events having the product name "Average number of photon scattering events" and no units declaration.
- The third and the forth lines of the header contain information on the selected spectral range and the number of output spectral points, respectively.

- The fifths header line contains the number of output altitude levels for weighting functions.
- The first data line contains the altitude grid used for the calculation of the weighting functions. Subsequently follow the blocks containing the weighting functions at different wavelengths for different measurement coordinates ordered in the same way as the radiances (see Section 3.23.1). Each block corresponds to an perturbation at the particular altitude level. The blocks are ordered according to the altitude grid written out in the first data line and separated by a blank line.

3.23.3 Air mass factors/Slant columns ("RTM Mode" is set to "amf" or "slant_col")

Air mass factors/slant columns of the selected atmospheric trace gas (see Section 3.1.4) are stored in "amf.dat" or "slant_col.dat", respectively. Additionally, "vert_col.dat" file is written out containing the vertical columns of the selected trace gas at appropriate local solar zenith angles. Files "amf.dat" or "slant_col.dat" have the same structure as "intensity.dat" (see Section 3.23.1). The second line of the header contains an appropriate product name only, no units declaration is required.

File "vert_col.dat" contains two data columns only, namely, the local solar zenith angle and appropriate vertical column of the selected trace gas.

3.23.4 Block air mass factors ("RTM Mode" is set to "block_amf")

Block air mass factors for the selected atmospheric trace gas (see Section 3.1.4) are stored in "block_amf.dat" file having the same structure as weighting function files (see Section 3.1.6) with an appropriate product name in the second header line.

3.23.5 Fluxes ("RTM Mode" is set to "flux")

The following products are written out:

- actinic flux ("act_flux.dat");
- upwelling and downwelling diffuse fluxes ("dif_flux_up.dat" and "dif_flux_dn.dat");
- upwelling scalar flux ("dif_scal_up.dat");
- upwelling and downwelling total fluxes ("total_flux_up.dat" and "total_flux_dn.dat");
- direct solar radiance ("dir_rad.dat").

All files have the same structure with an appropriate product name in the second header line. Let us consider the structure of output files if the calculations of fluxes were performed at altitudes 60 and 59 km (see Section 3.22.2), at solar zenith angles 50° and 70°, and at the wavelengths 500 and 550 nm.
An example of the "output_map.inf" file is given in this case as follows:

```
#  SCIATRAN 3.8.4 (DOM, plane-parallel mode, scalar RT)
#  Fluxes: dir_rad.dat, act_flux.dat, dif_flux_up.dat dif_flux_dn.dat
#          dif_scal_up.dat total_flux_up.dat total_flux_dn.dat
#  Num., solar zenith angle, altitude
```

```
1   50.00     60.0000
2   50.00     59.0000
3   70.00     60.0000
4   70.00     59.0000
```

The second and third columns contain the measurement coordinates where calculations of fluxes were performed. In particular, it is the solar zenith angle (50° and 70°) and altitudes (59 and 60 km). The structure of output file depends on the selection of "Output format for multiple wavelengths" control parameter (see Section 3.22.2).

If this control parameter is set to "wl_in_colm" then the structure of output file is given by

```
#  SCIATRAN 3.8.4 (DOM, plane-parallel mode, scalar RT)
#  Contents: Wavelength [nm], Upwelling diffuse flux [phot/s/cm^2/nm]
#  Irradiance: 1.0 [phot/s/cm^2/nm]
  500.00000   2.106164261E-001   2.106156899E-001   1.258248550E-001   1.258237499E-001
  550.00000   1.841254489E-001   1.841253057E-001   1.027466005E-001   1.027460266E-001
```

Here the calculated fluxes are written out in one line for each wavelength and sequence corresponds to the measurement coordinates given in the "output_map.inf" file.

If this control parameter is set to "wl_in_line" then the structure of output file is given by

```
#  SCIATRAN 3.8.4 (DOM, plane-parallel mode, scalar RT)
#  Contents: Wavelength [nm], Upwelling diffuse flux [phot/s/cm^2/nm]
#  Irradiance: 1.0 [phot/s/cm^2/nm]
    50.0000    60.0000   2.106164261E-001   1.841254489E-001
    50.0000    59.0000   2.106156899E-001   1.841253057E-001
    70.0000    60.0000   1.258248550E-001   1.027466005E-001
    70.0000    59.0000   1.258237499E-001   1.027460266E-001
```

Here the calculated fluxes are written out in one column for each wavelength and sequence corresponds to the measurement coordinates given in the "output_map.inf" file. The wavelengths do not present in this case.

Attention:

- If the "Intensity representation in output file" control parameter is set to "default" the output structure is the same as in the case of "wl_in_line".
- In the case of single wavelength the output structure is the same as in the case of multiple wavelengths.

3.23.6 Spherical albedo ("RTM Mode" is set to "spher_alb")

The reflected and transmitted spherical albedo ("spher_alb_up.dat", "spher_alb_dn.dat") are written out. Let us consider the structure of output files if the calculations of spherical albedo were performed at altitudes 60 and 59 km (see Section 3.22.2) at the wavelengths 500 and 550 nm.
An example of the "output_map.inf" file is given in this case as follows:

```
#  SCIATRAN 3.8.4 (DOM, plane-parallel mode, scalar RT)
#  Spherical albedo:  spher_alb_up.dat spher_alb_dn.dat
#  Num.,  altitude
   1     60.0000
   2     59.0000
```

The second column contains the measurement coordinates where calculations of spherical albedo were performed. It is the altitudes (60 and 59 km) in this case.
Files "spher_alb_up.dat" and "spher_alb_dn.dat" have the output structure which depends on the "Output format for multiple wavelengths" control parameter in the "control_out.inp" file. If this parameter is set to "wl_in_line" then:

- first two lines are header lines;
- the third line contains the wavelength grid;
- the spherical albedo data block starts from the fourth line. The first column of the data block contains the altitude grid and other columns contain values of the spherical albedo for all wavelengths.

An example of output structure of the file "spher_alb_up.dat" containing spherical albedo at two wavelengths 500 and 550 nm is given by

```
#  SCIATRAN 3.8.4 (DOM, plane-parallel mode, scalar RT)
#  Spherical albedo: reflection
                   500.00000          550.00000
     60.00000   3.344217264E-001   2.878242842E-001
     59.00000   3.344198413E-001   2.878235452E-001
```

If this parameter is set to "wl_in_colm" then :

- first two lines are header lines;
- the third line contains the altitude grid in [km];
- the spherical albedo data block starts from the fourth line. The first column of the data block contains the wavelength grid and other columns contain values of the spherical albedo for all altitudes.

An example of output structure of the file "spher_alb_up.dat" in this case is given as follows:

```
#  SCIATRAN 3.8.4 (DOM, plane-parallel mode, scalar RT)
#  Spherical albedo: reflection
                    60.00000           59.00000
    500.00000   3.344217264E-001   3.344198413E-001
    550.00000   2.878242842E-001   2.878235452E-001
```

Attention

- The structure of output files "spher_alb_up.dat" and "spher_alb_dn.dat" does not depend on the control parameter "Intensity representation in output file" in the "control_out.inp" file.
- In the case of single wavelength the output structure is the same as in the case of multiple wavelengths.

3.23.7 Vertical optical depth ("RTM Mode" is set to "vod")

Vertical optical depths of atmospheric trace gases are stored in the "tg_vod.dat" files. The first column of each of these files contains the wavelength and other columns contain corresponding optical depths for the selected atmospheric trace gases. If the optical depth depends on the solar zenith angle (e.g., for photochemically active species, see Section 3.12.2.5), results at all selected solar zenith angles (see Section 3.8.1) are written out. The assignment of data columns in "tg_vod.dat" is mapped in "output_map.inf" file containing the solar zenith angles and the trace gas names appropriate to each column in the optical depth file.

Additionally, if "RTM-CORE" is set to "DOM" (see Section 3.6), the "vod_all.dat" file is generated containing the wavelength in the first column and vertical optical depths for the Rayleigh scattering, aerosol scattering and absorption, cloud scattering and absorption, as well as the total optical depth (including gaseous absorption) in the subsequent columns.

3.23.8 Asymptotic intensity at TOA ("RTM-CORE" is set to "ASYMP")

The asymptotic intensity is stored in "intensity.dat" file in the same way as the intensity/radiance (see Section 3.23.1) with an appropriate product name in the second header line.

4 Retrieval using SCIATRAN

4.1 General information

Setting "RTM Mode" parameter to "ret" (see Sec. 3.1) the SCIATRAN program is switched to the retrieval mode. Depending on the selected type of the retrieval, this mode allows users to derive various atmospheric parameters from measured or simulated radiance spectra. The processing starts with the forward modeling using the input parameters selected for the radiative transfer model as described above. After the radiative transfer calculations are completed the simulated radiance and appropriate weighting functions are passed to the retrieval algorithm which estimates the desired atmospheric parameters appropriate to the spectrum supplied by the user. Due to non-linearity of most atmospheric problems an iterative process is usually applied resulting in the subsequent invoking of the radiative transfer model and retrieval algorithm. The retrieval algorithm is controlled by the parameters selected in "control_ret.dat". In most retrieval modes (see below, Sec. 4.2), the retrieval is performed in two stages. At the first retrieval stage also referenced to as the preprocessing, each line-of-sight defined in the "control_geom.inp" file (see Sec. 3.8) is processed independently. At this stage only scalar parameters are fitted, i.e., scaling factors for trace gas number density profiles, correction parameters, such as amplitudes of various spectral corrections and shift/squeeze coefficients (see Sec. 4.9), or any other scalar atmospheric or surface parameters. Although for some tasks, e.g., cloud top height retrieval, the pre-processing stage is sufficient to retrieve an atmospheric parameter of interests, generally the main retrieval is performed aimed to obtain altitude-dependent parameters such as vertical distributions of atmospheric species or optical parameters. Usually, the Optimal Estimation method (Rodgers, 2000) is employed as the default retrieval approach at the main retrieval stage. According to this approach the following equation has to be solved:

$$\hat{\mathbf{y}} = \mathbf{K}\hat{\mathbf{x}} + \epsilon\,, \tag{4.1}$$

where $\hat{\mathbf{y}}$ is the measurement vector containing in most retrieval modes the differences between logarithms of measured and simulated spectra, $\hat{\mathbf{y}} = \mathbf{y} - \mathbf{y_0}$, $\mathbf{K}$ is the linearized forward model operator represented by the weighting function matrix, $\hat{\mathbf{x}}$ is the state vector usually containing differences between the a priori and retrieved vertical distributions of atmospheric parameters, $\hat{\mathbf{x}} = \mathbf{x} - \mathbf{x_0}$, and ϵ represents errors of any kind. In the framework of the Optimal Estimation method the solution of Eq. (4.1) is found as

$$\mathbf{x} = \mathbf{x}_0 + \left(\mathbf{K}^T\,\mathbf{S}_y^{-1}\,\mathbf{K} + \mathbf{S}_a^{-1}\right)^{-1}\mathbf{K}^T\,\mathbf{S}_y^{-1}\,\left(\mathbf{y} - \mathbf{y}_0\right)\,, \tag{4.2}$$

where $\mathbf{S}_a$ is the a priori covariance matrix and $\mathbf{S}_y$ is the noise covariance matrix.

The information content of the measurements as well as the sensitivity of the retrieval can be analyzed using the averaging kernel and the solution covariance matrices obtained as

$$\mathbf{A} = \left(\mathbf{K}^T\,\mathbf{S}_y^{-1}\,\mathbf{K} + \mathbf{S}_a^{-1}\right)^{-1}\mathbf{K}^T\,\mathbf{S}_y^{-1}\,\mathbf{K} \tag{4.3}$$

and

$$\mathbf{S} = \left(\mathbf{K}^T \mathbf{S}_y^{-1} \mathbf{K} + \mathbf{S}_a^{-1}\right)^{-1} , \tag{4.4}$$

respectively (see (Rodgers, 2000) for details). The square roots of the diagonal elements of the solution covariance matrix are commonly referenced as the theoretical precision of the retrieval.

4.2 Type of the retrieval

Appropriate control file: "control_ret.inp"
Relevant control parameters: "Retrieval mode"

The type of the retrieval to be performed is controlled by the "Retrieval mode" parameter which defines the atmospheric parameters to be estimated from the spectrum supplied by the user as well as the way to use the supplied spectral information. The following retrieval modes are currently available:

- "tg" is the most general mode intended to retrieve the vertical distributions or vertical columns of atmospheric trace gases. In this retrieval mode the simulated spectral signal is fitted to the measured one using all measured spectral points and all line-of-sights in selected intervals. Depending on the settings made by user, the spectral fit can be performed either for absolute radiances of for differential signals. The shift and squeeze as well as other spectral corrections can be applied during the fit. More details on this retrieval mode can be found in (Rozanov, 2003; Rozanov et al., 2005, 2007).

- "triplet" is a special mode developed to retrieve vertical distributions of ozone using the triplet method (von Savigny et al., 2005c). The main idea of the triplet method is to combine the limb radiance profiles (i.e., observed limb radiances, $I(\lambda)$, as functions of the tangent height) averaged over 2 nm spectral intervals centered around λ_1=525 nm, λ_2=600, and λ_3=675 nm into the so-called Chappuis vector as $\ln\left[\frac{I(\lambda_2)}{\sqrt{I(\lambda_1)\, I(\lambda_3)}}\right]$. The averaging of the input spectra is performed over the spectral segments specified in the "Spectral segment info" input field (see Section 3.9). The radiative transfer modeling is performed only for the central wavelengths of each spectral segment which are used then to calculate the Chappuis vector. Thus, at least three spectral segments have to be specified to make use of the triplet method. The triplet method can be also extended to improve the retrieval quality in the upper stratosphere (above 40 km) considering also the UV radiance additionally to the Chappuis absorption band. The UV spectral segments have to be supplied before the triplet segments. The spectral radiance will be averaged within these segments and the logarithms of the resulting radiance profiles will be passed to the retrieval algorithm together with the Chappuis vector.

- "cth" is a special mode used to retrieve the cloud top heights from satellite measurements in the nadir viewing geometry using the O_2 absorption band between 758 and 772 nm.

- "tau_cld" mode is used to retrieve the cloud optical thickness. Using this mode one can estimate the cloud optical thickness at a given wavelength. The optical thicknes is single unknown parameter in this case. The input value is the reflectivity or intensity

of scattered radiation. If the input spectrum consist of a number of wavelengths the program will use the averaged reflectivity in the retrieval process.

- "ler" is a special mode used to retrieve the height of the effective Lambertian reflecting surface from satellite measurements in the nadir viewing geometry using the O_2 absorption band between 758 and 772 nm.
- "th_knee" mode can be used to retrieve the tangent height correction for satellite measurements of the scattered solar radiation performed in the limb viewing geometry. The retrieval is based on the analysis of the limb radiance profile shape between $\sim$ 40 km and $\sim$ 53 km tangent height in the spectral range from 295 to 305 nm. As a result one pointing correction value for all line-of-sights is obtained. The retrieval approach is described in details in (von Savigny et al., 2005a).
- All other retrieval modes are still under development and should not be activated.

4.3 Input data

Appropriate control files: "control_ret.inp"
Relevant control parameters: "Experimental data file", "Data step"

The name of the file containing measured or simulated spectra which will be used for the retrieval has to be specified in the "Experimental data file" input line. The file can contain an arbitrary number of header-lines starting with "#" or ";". The first column in the data file has to contain the wavelength in nm. Further columns are supposed to contain radiancies measured (or simulated) at different instrument line-of-sights. The total number of measurement data columns (i.e., excluding wavelength column) in the file has to be not less than the total number of the instrument line-of-sights specified for the forward modeling (as specified in viewing geometry settings, see Sec. 3.8.1).

Only spectral points within the spectral intervals defined in the "Spectral segment info" control field (see Sec. 3.9) are read from the data file. The original wavelength grid defined in the "Spectral segment info" control field is replaced by the wavelength grid of the measured spectra.

The "Data step" control field can be used to skip spectral points in the input file. For example, setting "Data step" to "3" each third spectral point from the input file will be used for the forward modeling and retrieval. The "Data step" parameter has to be set for each spectral segment (as defined in the "Spectral segment info" control field, see Sec. 3.9) independently, i.e., the number of the input values has to be not less than the number of selected spectral segments.

4.4 Selection of line-of-sights for retrieval

Appropriate control files: "control_ret.inp"
Relevant control parameters: "Tangent height selection",
"Start and end tangent heights"

If the "Tangent height selection" control parameter is set to "f" all line-of-sights from the input file (as defined in Sec. 4.3) will be used in the retrieval. Setting "Tangent height selection" to "t" only the line-of-sights within the specified range will be used. This can be useful, for example, in limb viewing geometry to exclude measurements at too low and too high tangent heights form the retrieval. The numbers of the start and the end line-of-sights defining the region to be used in the retrieval have to be specified in the "Start and end tangent heights" input field. The first line after the keyword defines the start and the second line the end line-of-sight number. Both numbers should be selected for each spectral segment independently, i.e., the number of values specified in the each input line has to be equal to the number of the selected spectral segments (see Sec. 3.9).

4.5 Reference spectrum

Appropriate control files: "control_ret.inp"
Relevant control parameters: "Reference spectrum", "Solar spectrum file", "Reference measurement number"

The "Reference spectrum" control line allows users to select a type of the reference spectrum to be used in the retrieval. All measured spectra selected for the retrieval (see Sec. 4.3 and 4.4) will be divided by the reference spectrum applying the shift and squeeze correction if required. The following selections can be done:

- "sol" - an extraterrestrial solar spectrum will be used as the reference. The name of the file containing the solar spectrum has to be specified in the "Solar spectrum file" input line. The file has to contain the wavelength in nm in the first column and the solar spectrum in the second column. The lines started with "#" or ";" at the beginning of the file are considered to be comment lines.
- "set" - a set of reference spectra, i.e., one spectrum per line-of-sight, will be considered. Thus, an its own reference spectrum has to be specified for each line-of-sight supplied in the measurement data file (as specified in the "Experimental data file" input line). The name of the file containing the reference spectra has to be specified in the "Solar spectrum file" input line. The file has to contain the wavelength in nm in the first column and the reference spectra in further columns. The number of the columns containing the reference spectra has to be equal to the number of data columns in the measurement data file (as specified in the "Experimental data file" input line). However, if the "Tangent height selection" control parameter is set to "t", only the reference spectra corresponding to the selected line-of-sights ("Start and end tangent heights" input field) will be considered.
- "los" - one of the line-of-sights contained in the measurement data file (as defined in Sec. 4.3) will be considered as the reference measurement. The number of the line-of-sight which is selected to be the reference measurement has to be specified in the "Reference measurement number" input field, i.e., the number selected here defines the column in the data file which will be considered to be the reference spectrum. The reference tangent height should be selected for each spectral segment independently, i.e., the number of values specified in the "Reference measurement number" input field has to be equal to the number of the selected spectral segments (see Sec. 3.9).

- "none" - no reference spectrum will be considered.

4.6 Profile or column?

Appropriate control files: "control_ret.inp"
Relevant control parameters: "Profile retrieval", "Retrieval mode"

Not used in "th_knee", "cth", and "ler" retrieval modes (see Sec. 4.2).

If the atmospheric trace gas amounts are retrieved ("Retrieval mode" is set to "tg" or "triplet", see Sec. 4.2), the "Profile retrieval" control line is used to select whether the vertical distribution or the vertical column will be retrieved. The selection is made for each trace gas independently. If a corresponding flag in the "Profile retrieval" control line is set to "f" the resulting profile will be obtained scaling the initial (a priori) profile. Otherwise concentrations at altitude levels defined by the input altitude grid (see Sec. 3.3) are retrieved.

4.7 Iterative approach

Appropriate control files: "control_ret.inp"
Relevant control parameters: "Iterations number limit"

To account for a non-linearity of the inverse problem an iterative approach is employed. This means that at each iterative step the forward model is initialized by the retrieval results from the previous iterative step. Thus the forward model and the retrieval block are run subsequently until the convergence is reached (see Sec. 4.7.2). The maximum number of iterations can be limited using the "Iterations number limit" control parameter.

4.7.1 Type of the iterative scheme

Relevant control parameters: "Use apriori information"

Not used in "th_knee", "cth", and "ler" retrieval modes (see Sec. 4.2).

If a corresponding flag in the "Use apriori information" control line is set to "t" the solution is found using the Gauss-Newton iterative scheme as described in (Rodgers, 2000):

$$\mathbf{x}_{i+1} = \mathbf{x}_0 + \left(\mathbf{K}_i^T \, \mathbf{S}_y^{-1} \, \mathbf{K}_i + \mathbf{S}_a^{-1}\right)^{-1} \mathbf{K}_i^T \, \mathbf{S}_y^{-1} \, \left(\mathbf{y} - \mathbf{y}_i + \mathbf{K}_i(\mathbf{x}_i - \mathbf{x}_0)\right) \, , \tag{4.5}$$

i.e., at each iterative step the solution is found as a deviation from the a priori state and the covariance matrix $\mathbf{S}_a$ is assumed to contain the covariances with respect to a priory state.

If for a particular atmospheric species no reliable a priory information (e.g., seasonal and zonal statistics and covariances) is available, one may do not want to constrain the global retrieval with values having no statistical meaning. In this case the Levenberg-Marquardt type of iterative process can be selected. This is done setting the corresponding flag in

the “Use apriori information” control line to “f”. In this case at each iterative step the a priori information is replaced by the results obtained at the previous iterative step and the covariance matrix $\mathbf{S}_a$ is assumed to contain the covariances with respect to this new state:

$$\mathbf{x}_{i+1} = \mathbf{x}_i + \left(\mathbf{K}_i^T \mathbf{S}_y^{-1} \mathbf{K}_i + \mathbf{S}_a^{-1}\right)^{-1} \mathbf{K}_i^T \mathbf{S}_y^{-1} \left(\mathbf{y} - \mathbf{y}_i\right) , \tag{4.6}$$

This approach regularize the retrieval at each iterative step but allows the resulting profiles to deviate from a priori state unlimited.

4.7.2 Convergence criteria

Appropriate control files: “control_ret.inp”
Relevant control parameters: “Convergence criteria”, “Convergence altutude region”, “Convergence for gas”

The convergence of the iterative process is controlled using two criteria specified in the “Convergence criteria” control line. The first value controls the relative change of the root mean square of the fit residual, i.e., RMS_NEW/RMS_OLD - 1, and the second value controls the relative change of the retrieved parameters. For the retrieval of atmospheric trace gas vertical distributions, the relative change of the retrieved parameters is defined as the maximum change in the number densities at all altitude levels between the lower and the upper altitudes specified in the “Convergence altitude region” control line for the atmospheric species selected in the “Convergence for gas” input line or for all trace gases included in the retrieval if the “Convergence for gas” control parameter is set to “All”.

The iterative process is stopped if one of the relative changes is below the selected threshold.

4.8 Regularization

Appropriate control files: “control_ret.inp”

4.8.1 A priori covariance matrix

Relevant control parameters: “Apriori information”, “Correlation radius”

Only used in “tg” and “triplet” retrieval modes (see Sec. 4.2).

The “Apriori information” control line is used to set diagonal elements of the a priori covariance matrix in the trace gas retrieval modes (“Retrieval mode” is set to “tg” or “triplet”, see Sec. 4.2). The values to be set are the relative variances, i.e., a selected value of ”0.4” means a relative variance of 40%. The diagonal elements of the a priori covariance matrix, $\mathbf{S}_a$, are calculated as squares of the relative variance values. The variances are to be set for each gas independently and supposed to be altitude independent.

The off-diagonal elements of the a priori covariance matrix are defined using the "Correlation radius" input field as follows:

$$\mathbf{S}_a^{i,j} = \sigma^2 \exp\left[-\frac{|z_i - z_j|}{r_c}\right] , \tag{4.7}$$

where σ are the variances defined in the "Apriori information" control line, z_i and z_j are the altitudes corresponding to the element (i,j) of the covariance matrix, and r_c is the correlation radius specified in the "Correlation radius" input field. No correlation between the concentrations of different trace gases can be set.

4.8.2 Tikhonov regularization

Relevant control parameters: "Tikhonov parameter"

Only used in "tg" and "triplet" retrieval modes (see Sec. 4.2).

The Tikhonov regularization is used to constrain the smoothness of the retrieved profiles. If Tikhonov regularization is turned on, the statistical regularization matrix, which is normally represented by an inverse a priori covariance matrix, is extended by the Tikhonov matrix. Thus, for example, in the case of the Newtonian iterative scheme, the solution is found as

$$\mathbf{x}_{i+1} = \mathbf{x}_0 + \left(\mathbf{K}_i^T \mathbf{S}_y^{-1} \mathbf{K}_i + \mathbf{S}_r\right)^{-1} \mathbf{K}_i^T \mathbf{S}_y^{-1} \left(\mathbf{y} - \mathbf{y}_i + \mathbf{K}_i(\mathbf{x}_i - \mathbf{x}_0)\right) , \tag{4.8}$$

where

$$\mathbf{S}_r = \mathbf{S}_a^{-1} + \mathbf{S}_t^T \mathbf{S}_t \tag{4.9}$$

and $\mathbf{S}_t$ is a first order derivative matrix weighted by an appropriate parameter which will be referred to as the Tikhonov parameter.

The Tikhonov parameters are set for each trace gas independently in the "Tikhonov parameter" input field. The first line in the control field defines the number of the atmospheric species which a Tikhonov parameter will be set for. If the first line contains zero, the Tikhonov regularization will be turned off. Each of the subsequent lines have to contain the trace gas name and the value of the Tikhonov parameter to be used for this gas. The number of the subsequent lines has to be equal to the number specified in the first line of the input field. All lines below are ignored. Tikhonov parameters for all trace gases not mentioned in the "Tikhonov parameter" input field are set to zero, i.e., no constrains with respect to the smoothness of the retrieved profiles are introduced for these species.

Limitation:

- Tikhonov regularization should not be used together with the Information Operator approach (see Sec. 4.14).

4.8.3 Noise covariance matrix

Relevant control parameters: "Signal to Noise ratio mode", "S/N ratio correction factor", "S/N ratio", "S/N ratio file"

Not used in “cth” and “ler” retrieval modes (see Sec. 4.2).

The measurement noise is assumed to be uncorrelated and is described by a diagonal noise covariance matrix. Depending on the mode selected in the “Signal to Noise ratio mode” input field, diagonal elements of the noise covariance matrix are calculated using a constant user defined value, read from the file, or estimated from the residuals. Setting “Signal to Noise ratio mode” to “C” a constant signal to noise ratio specified in the “S/N ratio” input field is used for all measurement points. If “Signal to Noise ratio mode” is set to “R” the signal to noise ratios are read from the file. The appropriate filename should be specified in the “S/N ratio file” control line. The input file has to contain the wavelength in the first column and one data column per line-of-sight (as specified in viewing geometry settings, see Sec. 3.8.1) containing the signal to noise ratios, i.e., the total number of the columns in the file has to be as large as the number of output line-of-sights according to “control_geom.inp” plus one. Setting “Signal to Noise ratio mode” to “E” the signal to noise ratio is estimated from the fit residuals obtained at the preprocessing step after the shift and squeeze as well as all selected spectral corrections are applied (see Sec. 4.9). The signal to noise ratio is estimated for each line-of-sight and each spectral segment independently. This approach is only available in “tg” retrieval mode (see Sec. 4.2) if all flags in the “Perform shift and squeeze” input field are set to “t” (see Sec. 4.9). Estimated values of signal to noise ratio can be changed using the “S/N ratio correction factor” input field, i.e., the signal to noise ratios estimated from the residuals are multiplied by the factor set in this input field.

4.9 Spectral corrections

Appropriate control files: “control_ret.inp”
Relevant control parameters: “Perform shift and squeeze”, ”Number of correction spectra”, “Correction spectra file names and shift mode”, ”Offset correction”, “Perform squeeze”

Available only in “tg”, “cth”, and “ler” retrieval modes (see Sec. 4.2). You need the GALAHAD Quadratic Programming library installed on your computer to use this mode.

All spectral corrections are applied at the pre-processing step using the scaling factors obtained from the shift-squeeze routine. Thus, this can only be done if shift and squeeze correction is activated, i.e., the corresponding flag in the “Perform shift and squeeze” input line is set to “t”, otherwise the entire pre-processing step is skipped. The flags are set for each spectral segment (as defined in the “Spectral segment info” control field, see Sec. 3.9) independently. If the shift-squeeze correction is turned on, the shift and squeeze of the reference spectrum with respect to the measured spectrum (input data), the shift and squeeze of the modeled spectrum (resulted from the forward model run) with respect to the measured spectrum as well as shift, squeeze and scaling factors for the spectral corrections are derived from the spectral fit. This is done for each line-of-sight and each spectral segment independently. Setting flags in the “Perform squeeze” control line to “f” the squeeze of the correction spectra, of the reference spectrum with respect to the measured spectrum, and of the modeled spectrum with respect to the measured spectrum, respectively, will not be performed, i.e., the appropriate spectra will be only shifted with respect to each other.

The number of the spectral corrections to be included in the spectral fit is specified in the “Number of correction spectra” control line. Each spectral correction has to be supplied as

a separate file. Each file has to contain the wavelength in nm in the first column and the spectral correction in the second column. The lines started with "#" or ";" at the beginning of the file are considered to be comment lines. The file names are specified in the "Correction spectra file names and shift mode" input field. Each filename has to be followed by the label "I", "M", "S", or "N" determining the behavior of the corresponding correction in the spectral fit. Setting the label to "I" denotes that shift and squeeze for this spectral correction will be done independently of all other spectra included in fit. Labels "M" or "S" denote that the spectral correction will be shifted/squeezed by the same amount as the model or reference (solar) spectrum, respectively. Setting the label to "N" the wavelength grid of the spectral correction will not be changed, i.e., no shift and squeeze will be applied. Nevertheless, the scaling factor for the spectral correction labeled with "N" will be estimated.

A special correction is introduced setting the "Offset correction" control parameter to "t". In this case the reference spectrum is assumed to have a wavelength independent offset which can be caused, for example, by the stray light, i.e.,

$$\tilde{I}_0(\lambda) = I_0(\lambda) + I_c\,. \tag{4.10}$$

Since the spectral fit is performed for logarithms of signals:

$$\ln \tilde{I}_0(\lambda) = \ln(I_0(\lambda) + I_c) \approx \ln I_0(\lambda) + \frac{I_c}{I_0(\lambda)}\,, \tag{4.11}$$

where only first two terms of the Tailor expansion of $\ln(I_0(\lambda) + I_c)$ are considered and $I_c \ll I_0(\lambda)$ is assumed. Thus the offset correction is performed including the $1/I_0(\lambda)$ term in the spectral fitting. The shift and squeeze for the offset correction is always equal to that of the reference spectrum.

4.10 Subtraction of a polynomial and spectral smoothing

Appropriate control files: "control_ret.inp"
Relevant control parameters: "Polynomial extraction", "Polynomial order", "Smoothing parameter"

Available only in "tg", "cth", and "ler" retrieval modes (see Sec. 4.2).

If the "Polynomial extraction" flag is set to "t" a polynomial will be subtracted from all spectral signals and weighting functions included in the fit, i.e., only the differential signals will be used. The polynomial order is specified in the "Polynomial order" input line. Both parameters need to be specified for each spectral segment (as defined in the "Spectral segment info" control field, see Sec. 3.9) independently. The "Smoothing parameter" control parameter allows user to smooth all input spectra before the spectral fit. The smoothing is done using the forward and backward Fourier transformation. The input parameter corresponds approximately to the number of spectral points to be averaged. If "Smoothing parameter" is set to "1" no spectral smoothing is performed.

4.11 Maximum retrieval height

Appropriate control files: "control_ret.inp"
Relevant control parameters: "Set maximum retrieval height",
"Maximum retrieval height"

These settings are only used in the trace gas retrieval modes ("Retrieval mode" is set to "tg" or "triplet", see Sec. 4.2) for the atmospheric species whose vertical distributions are to be retrieved, i.e., if the appropriate flag in the "Profile retrieval" control line is set to "t" (see Sec. 4.6). The default setting of the "Set maximum retrieval height" control parameter is "off". In this mode vertical profiles of the atmospheric trace gases are retrieved over the entire altitude range, i.e., from the bottom to the top of the atmosphere. Otherwise the maximum retrieval height is introduced, above which the a priori variances for all retrieved species are set to 1%. If "Set maximum retrieval height" is set to "read" the maximum retrieval height in km will be read from the "Maximum retrieval height" control field. The "auto" mode can only be used in the limb viewing geometry if the "Type of LOS definition" control parameter in "control_geom.inp" file is set to "th" (see Sec. 3.8.1). In this mode the maximum retrieval height is set to the tangent height of the uppermost line-of-sight selected for the retrieval (see Sec. 4.4).

4.12 Dark current correction

Appropriate control files: "control_ret.inp"
Relevant control parameters: "Dark current correction", "Dark current column"

Assuming that the measurement at one of the line-of-sights contains no useful information but just instrument dark current signal or stray light and this interfering signal does not change much from one line-of-sight to other, one may want to make an additional correction subtracting this signal from the measurements at other line-of-sights. This mode is activated setting the "Dark current correction" control parameter to "t". The number of the data column which will be subtracted from all other data columns has to be specified in the "Dark current column" control field. Please be careful, setting this number to a value larger than the total number of the measurement data columns in the input file leads to wrong retrieval results with no error message.

4.13 Do you want to re-run the forward model?

Appropriate control files: "control_ret.inp"
Relevant control parameters: "Calculate model spectrum", "Model spectrum directory"

Available only in "tg" and "triplet" retrieval modes (see Sec. 4.2).

In the retrieval mode the initial state of the atmosphere as well as the modeled intensities and weighting functions are stored in the auxiliary files after every run of the radiative transfer model. This files are stored in the "DATA_OUT" subdirectory and identified by the "_unformatted" label. Dealing with a retrieval parameter optimization task one do not need

to re-run the radiative transfer model for the same atmospheric state and can use the data stored at previous forward model run instead. This can be done setting the "Calculate model spectrum" control parameter to "f". Please note, you must not change any forward model settings in "control.inp" or "control_geom.inp" files if you do not re-run the forward model. Furthermore, if you perform more then one iteration in this mode the stored data will NOT be replaced after the forward model run at subsequent iterations.

The default location of the auxiliary files can be changed using the "Model spectrum directory" control line. Please note, this line specifies only the directory which the auxiliary files will be read from. The default location for the writing of the files can not be changed.

4.14 Information Operator approach

Appropriate control files: "control_ret.inp"
Relevant control parameters: "Eigenvectors decomposition", "Threshold for eigenvalues", "Eigenvectors decomposition with constraints"

Not available in "cth" and "ler" retrieval modes (see Sec. 4.2).

If the trace gas retrieval mode is selected, i.e., the "Retrieval mode" control parameter is set to "tg", the Information Operator approach can be used instead of the Optimal Estimation method to obtain the vertical distributions or total columns of atmospheric trace gases. In this case the solution is projected to the space spawned by the eigenvectors of the information operator defined by $\mathbf{P} = \mathbf{S}_a \, \mathbf{K}^T \, \mathbf{S}_y^{-1} \, \mathbf{K}$. At each iterative step the solution is found as eigenvector series expansion,

$$\mathbf{x}_{i+1} - \mathbf{x}_0 = \sum_{k=1}^{N_i} \beta_{i,k} \psi_{i,k} \; , \tag{4.12}$$

with the expansion coefficients

$$\beta_{i,k} = \frac{\lambda_{i,k}}{n_{i,k} \, (1 + \lambda_{i,k})} \, \psi_{i,k}^T \, \mathbf{K}_i^T \, \mathbf{S}_y^{-1} \, \Big[\mathbf{y} - \mathbf{y}_i + \mathbf{K}_i (\mathbf{x}_i - \mathbf{x}_0) \Big] \; , \tag{4.13}$$

where $\psi_{i,k}$ and $\lambda_{i,k}$ are the eigenvectors and the corresponding eigenvalues of the information operator $\mathbf{P}$, correspondingly, N_i is the number of the significant eigenvectors, and $n_{i,k}$ is defined by the following scalar product:

$$n_{i,k} = \langle \mathbf{K}^T \, \mathbf{S}_y^{-1} \, \mathbf{K} \, \psi_{i,k} \, , \, \psi_{i,k} \rangle \; . \tag{4.14}$$

Only the eigenvectors, whose eigenvalues are larger than or equal to the value specified in the "Threshold for eigenvalues" control field, are considered to be significant. The default value of the "Threshold for eigenvalues" control parameter is 1.0. The dimension of the basis in the projection space is defined by the number of the significant eigenvectors and, thus, is determined by the information content of the measurements. The main advantage of this method is an additional noise filtering due to a rejection of statistically insignificant components of the solution. However, because of inappropriate settings of measurement noise and a priory covariances or a presence of systematic (non-Gaussian) errors the method to select the significant eigenvectors may fail leading to a loss of a vertical structure information in the

solution. More details on the Information Operator approach can be found in (Hoogen et al., 1999; Rozanov, 2003; Doicu et al., 2007). The Information Operator approach is switched on setting the "Eigenvectors decomposition" control parameter to "t".

Setting the "Eigenvectors decomposition with constraints" control parameter to "t" the solution can be constrained to avoid, for example, negative or too high values. Per default the constraints are set to avoid negative values in the retrieved profiles of atmospheric species. In the current version of the software, the constraints can only be changed in the source code. This control parameters is only used if "Eigenvectors decomposition" is set to "t" and ignored otherwise. The GALAHAD Quadratic Programming library must be installed to use the constraints.

Limitation:

- The Information Operator approach should not be used together with the Tikhonov regularization (see Sec. 4.8.2).

4.15 Outliers

Appropriate control files: "control_ret.inp"
Relevant control parameters: "Reject outliers", "Outlier criterion", "Perform shift and squeeze"

Available only in "tg", "cth", and "ler" retrieval modes (see Sec. 4.2).

Outliers are the spectral points having abnormally high values in the spectral fit residuals. Setting the "Reject outliers" control parameter to "t" this spectral points can be excluded from the fits. A criterion used to identify outliers is defined by the "Outlier criterion" control parameter. A spectral point is considered to be an outlier if the remaining spectral fit residual at this point is larger than "Outlier criterion" parameter multiplied by the root mean square of the residual. Since the outlier analysis is performed at the pre-processing retrieval stage, the outlier rejection can only be performed if the corresponding "Perform shift and squeeze" control parameter is set to "t" (see Sec. 4.9).

4.16 Gaussian noise generator

Appropriate control files: "control_ret.inp"
Relevant control parameters: "Noise generator"

For modeling studies, Gaussian noise generator can be used to add an additional normally distributed random noise to the radiance spectra contained in the input data files (selected using the "Experimental data file" control line, see Sec. 4.3). The noise generator is controlled by three input parameters selected in the "Noise generator" control field. Setting the first parameter in the input line to "t" the noise generator is switched on and a random noise sequence, S_N, is generated which is normally distributed and has a unity variance. This noise sequence is then scaled by the noise amplitude as defined by the second control parameter in

the "Noise generator" input line, A_N, and multiplied by the input spectrum, I. This product is then used as the noise, which is added to the input signal, i.e., $I_{noisy} = (1 + A_N S_N)I$. Thus, an input signal dependent noise is added to radiance spectra resulting in the signal to noise ratio of A_N^{-1} in the total signal. Although the generated noise sequence is random, it is always the same for different runs of the program. To obtain another noise sequence a series of values at the beginning of the generated sequence can be skipped. The number of noise points to be skipped is defined by the third parameter in the "Noise generator" control field. If the number of skipped values is larger than the total number of spectral points at all line-of-sights used in the forward model, a completely different noise sequence is obtained.

4.17 Cloud top height retrieval parameters

Appropriate control files: "control_ret.inp"
Relevant control parameters: "Retrieval mode"

All parameters described in this section are used in the cloud top height retrieval mode only, i.e., if the "Retrieval mode" control parameter is set to "cth" (see Sec. 4.2).

4.17.1 Cloud parameters to be retrieved

Relevant control parameters: "Number of geometrical parameters", "Geometrical cloud parameters"

The number of cloud parameters to be retrieved is defined by the 'Number of geometrical parameters" control parameter which can be set either to "1" or to "2". In the asymptotic mode, i.e., if the "RTM-CORE" is set to "ASYMP" (see Sec. 3.6.2) the "Number of geometrical parameters" control parameter must be set to "2". The cloud parameters to be retrieved have to be specified in the "Geometrical cloud parameters" input field. The following settings are valid:

- "Number of geometrical parameters" is set to "1":
  - "top" - the cloud top height (CTH) is retrieved whereas the cloud bottom height is fixed according to the input parameters in "cloud.inp" file (see Sec. 3.15);
  - "bot" - the cloud bottom height (CBH) is retrieved whereas the cloud top height is fixed according to the input parameters in "cloud.inp" file;
  - "thi" - both cloud top and bottom heights are retrieved whereas its geometrical thickness (CGT) is fixed according to the input parameters in "cloud.inp" file, i.e., the cloud is shifted vertically.
- "Number of geometrical parameters" is set to "2": any combination of "top", "bot", and "thi" has the same effect, i.e., both cloud top and bottom heights as well as its geometrical thickness are retrieved. Please note, that these parameters are not independent, i.e., CGT = CTH − CBH. The first parameter in the "Geometrical cloud parameters" control line is considered to be the primary retrieval parameter.

4.17.2 Constraints for cloud parameters

Relevant control parameters: “Geometrical thickness constraints”, “Cloud top height constraints”, “Cloud bottom height constraints”

The retrieval constraints are set by the “Cloud top height constraints”, “Cloud bottom height constraints”, and “Geometrical thickness constraints” control parameters defining the minimum (the first value in the control line) and the maximum (the second value in the control line) allowed values of the corresponding cloud parameters.

4.17.3 Lower reflection

Relevant control parameters: “Lower reflection”

The “Lower reflection” control parameter is used to reject cloud free scenes from the retrieval. This is done using the reflection function defined by $R = \frac{\pi I}{I_0 \cos(\Psi)}$, where I is the outgoing radiance backscattered from the Earth's atmosphere, I_0 is the solar irradiance, and Ψ is the solar zenith angle. If the reflection function calculated outside of the gaseous absorption bands is less than the minimum value defined by the “Lower reflection” control parameter, the cloud coverage is considered to be insufficient to retrieve cloud parameters.

4.17.4 Convergence criterion

Relevant control parameters: “CTH convergence criterion”

The convergence criterion for cloud parameter retrieval is defined by the “CTH convergence criterion” control parameter. The value should be specified in “km” and is valid for the primary retrieval parameter, i.e, the first parameter selected in the “Geometrical cloud parameters” control line. If the ”Number of geometrical parameters” control parameter is set to “2”, the convergence criterion for the secondary retrieval parameter is set as 2×“CTH convergence criterion”. The convergence is reached if one of the absolute differences between the cloud parameters found in the subsequent iterations is less than the corresponding convergence criterion.

4.18 Output files

Similar to the forward model output, all output files from the retrieval block are written out into the “./DATA_OUT/” subdirectory of main program directory.

4.18.1 Pre-processing stage

All output files described in this subsection are only written out if the verbosity level of the retrieval output (i.e., the second character in the "Verbosity level" control field, see Sec. 3.22.1) is set to "E" or "D".

During the pre-processing stage the output information is written out for each spectral segment and each line-of-sight independently and stored in the following files: "rad-mod-XX-YY", "mes-dat-XX-YY", and "ret_spec-XX-YY", where "XX" is the spectral segment number according to the "Spectral segment info" control field in the "control.inp" file (see Sec. 3.9) and "YY" is the line-of-sight number according to viewing geometry settings in "control_geom.inp". The numbering begins from "1". The line-of-sights are numbered as listed in "output_map.inf" file (see Sec. 3.23). The output files contain the following information:

- "rad-mod-XX-YY" contains simulated data resulting from the forward model run. The first column in the file contains the wavelength in "nm", the second column contains simulated radiance, and all subsequent columns contain the weighting functions of atmospheric parameters. In most retrieval modes both radiance and weighting functions are converted to the logarithmic representation, normalized with respect to the reference according to the setting in the "Reference spectrum" control field in "control_ret.inp" (see Sec. 4.5), and smoothed if necessary.
- "mes-dat-XX-YY" contains measured data read by the program from input files as specified in "control_ret.inp". The first column contains the wavelength in "nm", the second column contains the measured spectrum, and the third column contains the reference spectrum according to the setting in the "Reference spectrum" control field in "control_ret.inp". In most retrieval modes both measured and reference spectra are converted to the logarithmic representation and smoothed if necessary.
- "ret_spec-XX-YY" contains the fit results. The first column contains the wavelength in "nm", the second column contains the measured spectrum normalized to the reference spectrum (both spectra as in "mes-dat-XX-YY") with a relative shift/squeeze correction applied, the third column contains the simulated spectrum (as in "rad-mod-XX-YY") with a corresponding shift/squeeze correction applied, and all subsequent columns contain the weighting functions of fit parameters multiplied by the retrieved parameter values with corresponding shift/squeeze corrections applied. Thus, for a good fit, the difference between the normalized measured spectrum and the simulated spectrum, i.e., between the second and third data columns, should be close to the sum of all remaining columns, i.e., corrections identified by the fit procedure, differing only by the measurement noise. If necessary ("Polynomial extraction" control parameter in "control_ret.inp" is set to "t", see Sec. 4.10), the polynomial subtraction is performed for all data columns, except for the first one (wavelength grid).

Limitations:

- If the "Tangent height selection" control parameter in "control_ret.inp" is set to "t" (see Sec. 4.4) only the output information for the line-of-sights selected in the "Start and end tangent heights" control field is written out;
- If the "Perform shift and squeeze" control parameter in "control_ret.inp" is set to "f"

(see Sec. 4.9) no pre-processing is performed for the corresponding spectral segment and, thus, no output information is written out.

4.18.2 Retrieval results: Trace gas retrieval mode

In the trace gas retrieval mode ("Retrieval mode" control parameter is set to "tg" or "triplet", see Sec. 4.2) the following output files are generated during the main retrieval stage:

- The vertical distributions of atmospheric species resulted from the main retrieval are stored in "profiles_nd.dat" and "profiles_vmr.dat" files as number densities (molec/cm^3) and volume mixing ratios (ppV), respectively. Both files have the same format. The first four lines in each file are the header lines containing auxiliary information. The first header line contains the number of atmospheric species used in the retrieval. The second line contains the names of these species. The third header line contains "T" or "F" flag for each retrieved atmospheric species identifying if the vertical profile retrieval ("T") or a priori profile scaling ("F") was performed for this species. The fourth header line contains the vertical columns for each atmospheric species obtained integrating their vertical profiles over the entire altitude range. The header lines are followed by the vertical profile data block containing the altitude in "km" in the first column as well as three data columns (vertical profiles) for each atmospheric species. The order of species is the same as in the second header line. The first vertical profile represents the a priori information, and the second and third profiles are the results of the last but one and of the final iterative retrieval step, respectively (see Sec. 4.7).

- Additionally, the "ret_column.dat" file is written out containing the total columns (i.e., integrated vertical profiles) of all retrieved species. Three header lines at the beginning of this file contain exactly the same information about the retrieved species as in "profiles_nd.dat" and "profiles_vmr.dat" files. The fourth line contains the a priori total columns of the retrieved species (i.e., vertically integrated a priori profiles), whereas the fifth line contains the total columns after the retrieval (same as the fourth header line in "profiles_nd.dat" and "profiles_vmr.dat" files).

- Measured and simulated data as well as fit residuals before and after the last iterative retrieval step are stored in "pro_retr_pre.dat" and "pro_retr_rms.dat" files, respectively. The first line in both files contains the total number of the spectral points at all line-of-sights used in the retrieval process, i.e., the dimension of the measurement vector $\hat{\mathbf{y}}$ (see Sec. 4.1), the total number of spectral points in all spectral segments as specified in the "Spectral segment info" control field in "control.inp" (see Sec. 3.9), and the total number of line-of-sights according to viewing geometry settings in "control_geom.inp" (see Sec. 3.8). Please note, since some of spectral points as well as some of line-of-sights are not included in the retrieval, the first value is typically smaller than the product of the second and third values. Separated by empty lines above and below, the third header line contains the full wavelength grid as was used for the forward modeling according to "Spectral segment info" control field. The header lines are followed by the data block consisting of 5 columns. The first and the second data columns indicate the number of the line-of-sight and of the wavelength which the data points belong to, respectively. The line-of-sights are numbered as listed in "output_map.inf" file (see

Sec. 3.23). The wavelength numbering is appropriate to the wavelength grid given in the third header line. The third data column contains the fit residual. The fourth data column contains the pre-processed measured spectrum as it was used to create the measurement vector $\hat{\mathbf{y}}$ (see Sec. 4.1), i.e., all needed transformations are already performed and all corrections from the pre-processing stage are applied. The fifth data column contains the simulated spectrum including the contributions due to parameter changes at the current iterative retrieval step. Similar to the measured spectrum, all needed transformations are performed and all corrections from the pre-processing stage are applied.

- "wf_fit.dat" file contains the contributions of individual atmospheric species into the total simulated spectrum. The format of this file is similar to that of "pro_retr_*.dat" files. The first header line contains an additional value (fourth) giving the total number of atmospheric species included in the retrieval. The names of the retrieved species are listed in the second header line of "profiles_*.dat" files. The data block contains two numbering columns having the same meaning as in "pro_retr_*.dat" files and two spectral data columns per retrieved atmospheric species. The order of the retrieved species is as listed in the second header line of "profiles_*.dat" files. Each first column of spectral data contains the contribution into the total simulated signal due to initial concentrations of atmospheric species and each second column contains the contribution due to the retrieved differences in concentrations. Thus, the sum of two columns gives for each atmospheric species the full contribution of the retrieved vertical distribution into the simulated signal.

- "precision.dat" file contains the sequential number in the first column as well as diagonal elements of the solution and a priori covariance matrices in the second and the third columns, respectively (see Sec. 4.1 for details). The output order is as follows: first the covariance values for the first retrieved species at all retrieval altitudes are written out then the same for the second species and so on. The order of the retrieved species is as listed in the second header line and the altitude grid is the same as listed in the first column of "profiles_*.dat" files. The "precision.dat" file is not written out if the verbosity level of the retrieval output (i.e., the second character in the "Verbosity level" control field, see Sec. 3.22.1) is set to "N".

- "av_test.dat" file contains the averaging kernel matrix (see Sec. 4.1 for details). The order of the elements is the same as for "precision.dat" file. The "av_test.dat" file is not written out if the verbosity level of the retrieval output (i.e., the second character in the "Verbosity level" control field, see Sec. 3.22.1) is set to "N".

4.18.3 Retrieval results: Tangent height correction

In the tangent height correction mode ("Retrieval mode" control parameter is set to "th_knee", see Sec. 4.2) the retrieval results in one correction value which is written out to the "th_corr.dat" file as well as to the standard output (screen). The fit quality can be checked using "pro_retr_pre.dat" and "pro_retr_rms.dat" files which have the same format as described above (see Sec. 4.18.2).

4.18.4 Retrieval results: Cloud top height retrieval

In the cloud top height retrieval mode ("Retrieval mode" control parameter is set to "cth", see Sec. 4.2) the results are stored in "ret_parameter.dat" file. The file contains only one line listing the following parameters: latitude, longitude, surface elevation (height above sea level), surface albedo, solar zenith angle, cloud optical depth, cloud bottom height, cloud top height, cloud geometrical thickness, cloud fraction, root mean square from the spectral fit, cloud scene description, and retrieval quality flag.

4.18.5 Retrieval results: Height of the effective Lambertian reflecting surface

In the height of the effective Lambertian reflecting surface retrieval mode ("Retrieval mode" control parameter is set to "ler", see Sec. 4.2) the results are stored in "ret_parameter.dat" file, similar to the cloud top height retrieval mode. The file contains only one line listing the following parameters: latitude, longitude, retrieved height of the effective Lambertian reflector, surface albedo, solar zenith angle, and root mean square from the spectral fit.

4.18.6 Auxiliary files

All "*_unformatted.dat" files are used for temporary storage of the forward model output needed to re-run the retrieval without re-running the forward model (see Sec. 4.13). These files must not be changed or edited by users.

"xdiff_test.dat" contains the sequential numbering in the first column and the state vector resulting from the retrieval in the second column (see Sec. 4.1 for details). The order of elements is the same as for "precision.dat" file (sec Sec. 4.18.2). This is an intermediate product needed for control and debugging purposes.

If the Information Operator approach is used (see Sec. 4.14), the "evec.out" file contains significant eigenvectors of the Information Operator and the corresponding eigenvalues. The first line lists the number of the significant eigenvectors, the total length of the state vector (see Sec. 4.1 for details), and the maximum number of significant eigenvectors as set in the "Number of eigenvectors to be used" control field in "control_ret". Subsequently the eigenvalue-eigenvector blocks are written out (first eigenvalue then the corresponding eigenvector). The "evec.out" file is only written out if the verbosity level of the retrieval output (i.e., the second character in the "Verbosity level" control field, see Sec. 3.22.1) is set to "E" or "D".

A Tools to compile the GALAHAD Quadratic Programming Library for SCIATRAN >= 3.1

A.1 List of required modules/source files

All modules and corresponding source files needed to use the GALAHAD Quadratic Programming Library with SCIATRAN are listed in "needed_for_sciatran.txt" which can be downloaded at www.iup.physik.uni-bremen.de/sciatran/free_downloads. Additionally, the contents of the file are listed below.

```
src/smt/smt.f90:        MODULE GALAHAD_SMT_double
src/sils/sils.f90:      MODULE GALAHAD_SILS_double
src/sort/sort.f90:      MODULE GALAHAD_SORT_double
src/sym/symbols.f90:    MODULE GALAHAD_SYMBOLS
src/qpt/qpt.f90:        MODULE GALAHAD_QPT_double
src/qpp/qpp.f90:        MODULE GALAHAD_QPP_double
src/roots/roots.f90:    MODULE GALAHAD_ROOTS_double
src/rand/rand.f90:      MODULE GALAHAD_RAND_double
src/space/space.f90:    MODULE GALAHAD_SPACE_double
src/sbls/sbls.f90:      MODULE GALAHAD_SBLS_double
src/uls/uls.f90:        MODULE GALAHAD_ULS_double
src/spec/specfile.f90: MODULE GALAHAD_SPECFILE_double
src/scu/scu.f90:        MODULE GALAHAD_SCU_double
src/qpd/qpd.f90:        MODULE GALAHAD_QPD_double
src/fdc/fdc.f90:        MODULE GALAHAD_FDC_double
src/lsqp/lsqp.f90:      MODULE GALAHAD_LSQP_double
src/gltr/gltr.f90:      MODULE GALAHAD_GLTR_double
src/qpb/qpb.f90:        MODULE GALAHAD_QPP_double
```

A.2 Shell script to copy all needed source files

The shell script file "copy_for_sciatran.sh" can also be downloaded at www.iup.physik.uni-bremen.de/sciatran/free_downloads.

```
# Shell script to copy the GALAHAD quadratic programming library
# source files needed for SCIATRAN >= 3.1
```

```
# First argument is the name of the ouput directory
if [ "${1}" = "" ] ; then
    echo 'Output directory must be specified!'
    exit
fi

OUTPUT_DIR=${1}
mkdir $OUTPUT_DIR/SRC
filelist='sils/sils.f90 smt/smt.f90 qpt/qpt.f90 sort/sort.f90 sym/symbols.f90
qpp/qpp.f90 roots/roots.f90 qpd/qpd.f90 rand/rand.f90 sbls/sbls.f90 space/space.f90
uls/uls.f90 spec/specfile.f90 scu/scu.f90 lsqp/lsqp.f90 fdc/fdc.f90 gltr/gltr.f90
qpb/qpb.f90'

for file in $filelist; do
    cp src/$file $OUTPUT_DIR/SRC/
done

exit
```

A.3 Makefile

The Makefile supports currently Intel Fortran Composer (ifort), gfortran, g95, and xlf (IBM) compilers and can be easily extended for use with any other Fortran compiler. This file can also be downloaded from www.iup.physik.uni-bremen.de/sciatran/free_downloads

```
############################################################################
#
# Makefile to compile the GALAHAD quadratic programming library
# for the SCIATRAN software package
#
############################################################################
ht = $(HOSTTYPE)
ifeq ($(ht),)
    ht=unknown
endif

objdir = OBJ_$(ht)_$(fc)
testdir := $(shell ls -d $(objdir) 2> /dev/null)
OBJDIR = ./$(objdir)/
FC = $(fc)

ifeq ($(fc),ifort)
   FFLAGS  =  -O3 -module $(OBJDIR) -u -w95
   F77_FLAGS = $(FFLAGS)
endif
```

```
ifeq ($(fc),g95)
   FFLAGS  =  -O3 -fmod=$(OBJDIR) -fimplicit-none -Wall
   F77_FLAGS = $(FFLAGS)
endif
ifeq ($(fc),gfortran)
   FFLAGS  =  -O3 -J$(OBJDIR) -I$(OBJDIR) -fimplicit-none -Wall
   F77_FLAGS = $(FFLAGS)
endif
ifeq ($(fc),xlf95_r)
   FFLAGS  = -O3 -qnoipa -q64 -qsmallstack -qmoddir=$(OBJDIR) -I$(OBJDIR)
   F77_FLAGS = -qfixed $(FFLAGS)
endif

OBJECTS_GALAHAD = $(OBJDIR)/smt.o $(OBJDIR)/sils.o $(OBJDIR)/sort.o \
$(OBJDIR)/symbols.o $(OBJDIR)/qpt.o $(OBJDIR)/qpp.o $(OBJDIR)/roots.o \
$(OBJDIR)/rand.o $(OBJDIR)/space.o $(OBJDIR)/uls.o $(OBJDIR)/specfile.o \
$(OBJDIR)/sbls.o $(OBJDIR)/scu.o $(OBJDIR)/qpd.o $(OBJDIR)/fdc.o \
$(OBJDIR)/lsqp.o $(OBJDIR)/norms.o $(OBJDIR)/gltr.o $(OBJDIR)/qpb.o

OBJECTS_HSL = $(OBJDIR)/ma27.o

all: setup $(OBJECTS_GALAHAD) $(OBJECTS_HSL)
ar rc $(OBJDIR)/libgalahad.a $(OBJECTS_GALAHAD) $(OBJECTS_HSL)
rm $(OBJECTS_GALAHAD) $(OBJECTS_HSL)

setup:
ifeq ($(ht),unknown)
@echo "Host type is not recognized (set to 'unknown')"
endif
ifeq ($(testdir),)
mkdir $(objdir)
endif

$(OBJECTS_GALAHAD): $(OBJDIR)%.o : SRC%.f90
$(FC) -c -o $@ $(FFLAGS) $<

$(OBJECTS_HSL): $(OBJDIR)%.o : SRC%.f
$(FC) -c -o $@ $(F77_FLAGS) $<

clean:
rm $(OBJDIR)/*.o
rm $(OBJDIR)/*.mod
rm $(OBJDIR)/*.a

#######################################################################
#
# End of Makefile
```

```
#
#########################################################################
```

B Keyword reference list

B.1 "control_ac.inp"

B.2 "control_aer.inp"

B.3 "control_brdf.inp"

B.4 "control_conv.inp"

B.5 “control_geom.inp”

B.6 “control_la.inp”

B.7 “control_out.inp”

B.8 "control_pas.inp"

B.9 "control_prof.inp"

B.10 "control_ray.inp"

B.11 "control_ret.inp"

B.12 "control_rrs.inp"

B.13 "control_te.inp"

B.14 "control_uwt.inp"

B.15 "control_wf.inp"

B.16 "control.inp"

B.17 "cloud.inp"

B.18 Other control files

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