

**User's Guide for the
Software Package SCIATRAN
(Radiative Transfer Model and
Retrieval Algorithm)**

- Version 2.2 -

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Chapter 1

Introduction

1.1 General

This user's guide describes how SCIATRAN 2.2 software package can be installed and run on UNIX/LINUX workstations and PCs. The program can also be installed under Microsoft WINDOWS, however, we can not offer any installation/execution support for WINDOWS users.

It is strongly recommended to read carefully this user's guide before starting to use SCIATRAN.

SCIATRAN 2.2 is a software package incorporating a radiative transfer model and a retrieval algorithm which can be easily adjusted to solve a wide range of scientific tasks. The program has been developed at the Institute of Remote Sensing/Institute of Environmental Physics (*iup/ife*), University of Bremen, Bremen, Germany.

SCIATRAN Version 2.2 is a result of a further development of the SCIATRAN 2.0 radiative transfer model [36] which was an extension of the SCIATRAN 1.2 [39].

SCIATRAN has been developed in FORTRAN 95. Following computer architectures are supported: COMPAQ Alpha (tested on: DS20, XP1000; SuSE Linux 7.0, Gentoo Linux; COMPAQ fort compiler), SUN (tested on: Blade 1000; Solaris; SUN Workshop F95 compiler), PC (tested on: Intel Pentium IV, Intel Pentium-M, Intel Core2 Duo, AMD 2800+, AMD Opteron; SuSE Linux 9.x, 10.x; INTEL ifort \geq 8.1 compiler), IBM (tested on: Regatta; AIX; xlf95_r compiler). For other computer platforms/compiler an appropriate adaptation of Makefile by user is required.

Please be advised, *ife/iup* **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 <http://www.iup.physik.uni-bremen.de/sciatran>).

SCIATRAN has been designed to allow fast and accurate simulation of radiance spectra as measured from space with the passive remote sensing UV-Vis-NIR spectrometers GOME¹ [10] (spectral range: 240-790 nm; viewing mode: nadir) and SCIAMACHY² [2] (240-2400 nm; nadir,

¹Global Ozone Monitoring Experiment

²Scanning Imaging Absorption spectroMeter for Atmospheric CHartographY

limb, solar and lunar occultation). Furthermore, the program can be used to model ground-based and air-borne measurements as well as to calculate corresponding air mass factors. 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 thesis generated demonstrating that SCIATRAN is a valuable tool to be used for many applications [37, 38, 33, 30, 26, 47, 4, 24, 22, 43, 34] , such as the retrieval of atmospheric constituents from remote radiance measurements, calculation of air mass factors and slant columns of atmospheric trace gases, cloud top height retrieval. Many of these papers also contain comparison with other models or measurements. Therefore, we consider this model to be sufficiently validated. Nevertheless, validation is a never ending and still ongoing task, especially important when applying the program to "new" areas or after program modification.

1.2 Features overview

Products:

Modeling: radiance/intensity, weighting functions, air mass factors (AMF), slant columns, vertically resolved AMFs (block AMFs), fluxes (actinic, upwelling, downwelling, diffuse and total), spherical albedo, vertical/slant optical depth.

Retrieval: trace gas vertical profiles, cloud top height, tangent height correction.

Wavelength range:

Basically 175.44 nm - 2400 nm, several spectral windows can be selected. The sub-range fully supported (e.g., by correlated- k parameters, see below) is 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) with an extension to a shorter UV range down to 175.44 nm which is useful for calculations of heating rates or photolyze frequencies.

Geometry:

Any observation geometry as well as any position of the instrument in the space, on the ground, or in the atmosphere which is common for spectral measurements of the scattered solar light is supported by SCIATRAN. Although, some of the program features are limited to certain observation modes.

Atmospheric model:

Trace gases (O₃, NO₂, ClO, OClO, BrO, HCHO, SO₂, NO₃, O₄, O₂, H₂O, CO₂, CO, CH₄, and N₂O), aerosols, clouds.

Earth surface:

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

New features in SCIATRAN 2.x with respect to SCIATRAN 1.2:

- Program is written in FORTRAN 95.
- Spherical mode added (can be used for solar zenith angles up to 98 deg). User can switch between the pseudo-spherical and the spherical mode.
- All viewing geometries supported (nadir, off-nadir, zenith-sky, off-axis, limb).
- Any observer position supported (TOA, BOA, any point within and above the atmosphere).
- Field of view integration in spherical mode.
- Extended spectral region: 175 - 2400 nm.
- Spectral data base for “line-absorbers” (including c-k distribution scheme) is updated to HITRAN 2004.
- New spectral data base for optical parameters of water clouds.
- Photochemically active species can be considered in spherical mode.
- New radiative transfer core (based on the discrete-ordinates method).
- Extremely fast quasi-asymptotical approach to calculate reflected radiation in a cloudy atmosphere within “line-absorber” (O₂, H₂O, etc.) spectral bands.
- Linearization (weighting functions) with respect to a variety of atmospheric parameters (trace gas concentrations, pressure, temperature, Rayleigh scattering, aerosol and cloud parameters).
- Incorporated retrieval block based on either Optimal Estimation or Information Operator approach (alternatively).
- Parallel computation on SMP systems (Open MP standard).

New features in SCIATRAN 2.1 with respect to SCIATRAN 2.0:

- Solar occultation mode is added allowing the modeling of the solar/lunar radiation transmitted through the Earth’s atmosphere.
- Retrieval block is included in the software package which can be used to derive a variety of atmospheric parameters from the measurement of the scattered or transmitted solar radiation. However, some of retrieval modes require the NAG FORTRAN Library (commercial).
- Multiple viewing angles and solar zenith angles are now allowed in the discrete ordinate mode.
- Discrete ordinate solver can be run in the pseudo-spherical mode. Refraction can be accounted for.

- A new adaptive altitude grid technique can be used in the discrete ordinate mode resulting in a substantial reduce of the calculation time without a considerable loss of the accuracy.
- Aerosol extinction and absorption coefficients as well as asymmetry coefficients for aerosol phase function (Henyey-Greenstein type) can be specified manually.

New features in SCIATRAN 2.2 with respect to SCIATRAN 2.1:

- Discrete ordinate solver is now available in all observation modes including the spherical geometry.
- The full set of weighting functions is now available in the spherical mode (if the discrete ordinate solver is used).
- Clouds can be considered in limb viewing geometry (spherical shell clouds only).
- The commercial NAG FORTRAN library was replaced by the GALAHAD library (see <http://galahad.rl.ac.uk/> for detials) which is freely available for “Academic” use.

Open issues:

- Not implemented are non-thermal (non-LTE) emissions such as the NO- γ band emissions around 260 nm or the O₂(a¹ Δ_g) emission around 1.27 nm.
- The pressure dependence of all absorption cross-section (except of line-absorber) is presently neglected in the pressure weighting function.

Temporary unavailable features:

- Rotational Raman scattering.

Chapter 2

Quick Start

2.1 Supported computer systems

- g95: we have encountered problems then trying to link the lapack/blas libraries using g95 compiler. Please inform us if you were successful compiling SCIATRAN using g95.
- COMPAQ Alpha, SuSE 7.0 or Gentoo Linux, COMPAQ “fort” Compiler
- SUN (tested on Blade 1000), Sun Workshop Compiler
- PC under Linux , Intel “ifort” Compiler.
 - SCIATRAN 2.2 is known to work on: Intel Pentium IV, Intel Pentium M, Intel Core2 Duo, AMD Opteron; SuSE Linux 9.x, 10.x; ifort 8.1, 9.0.
 - For older AMD processors you may want to read the instructions written by Thomas Nauss (University of Marburg) describing an installation of SCIATRAN on the following computer system: AMD Athlon XP 2800+, SuSE Linux 9.0. (<http://www.iup.physik.uni-bremen.de/sciatran/amd.html>)
- IBM Regatta, “xlf_r” Compiler
- For any other system an appropriate adjustment of Makefile by user is required.
- SCIATRAN 2.2 is also reported to work under Microsoft WINDOWS, amongst others with cygwin. Some instructions how to operate SCIATRAN under Microsoft WINDOWS witten by other users can be found at the SCIATRAN web page (<http://www.iup.uni-bremen.de/sciatran/sciatran2xquickstart>). Unfortunately, we cannot offer any instalation or execution support for WINDOWS users.

2.2 Software requirements

- Any FORTRAN 95 Compiler

- LAPACK and BLAS FORTRAN libraries (<http://netlib.org/lapack>)
- Optionally: 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 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 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 GALAHAD files needed for SCIATRAN will be placed to, e.g., “`bash copy_for_sciatran.sh YOUR_GALAHAD_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_GALAHAD_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_GALAHAD_DIR/SRC`” directory.

- Create (or download) the `Makefile` as described in Sec. A.3, in the “*YOUR_GALAHARD_DIR*” directory. The current version of the `Makefile` supports only “`ifort`” (PC) and “`xlf`” compilers. For other compilers the `Makefile` must be adapted appropriately.
- Change to the “*YOUR_GALAHARD_DIR*” directory.
- Create a subdirectory named “`OBJ_{COMPILER_NAME}`” where the GALAHAD library file, module files, as well as temporary object files will be stored, e.g., for “`ifort`” compiler type “`mkdir OBJ_IFORT`”.
- Type “`gmake`” to compile the library. This will create a library file named “`libgalahad.a`” as well as several module files (“`*.mod`”) which will be placed in the “`OBJ_{COMPILER_NAME}`” subdirectory. 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).

2.4 How to install SCIATRAN

- Download SCIATRAN 2.2 (`sciatran-2.2.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 2.2 (`sciatran-2.2.X.tgz`):
 - type “`sciatran-2.2.X.tgz`”, file `sciatran-2.2.X.tar` will be created;
 - type “`tar xvpf sciatran-2.2.X.tar`”, a subdirectory `Execute-2.2` will be created;
 - remove `sciatran-2.2.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-2.2.X.tar` file.
- Change to `Execute-2.2` 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 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_GALAHAD_DIR/OBJ_IFORT -u -w95
LNFLAGS = $(FFLAGS) -L YOUR_GALAHAD_DIR/OBJ_IFORT -lgalahad -llapack_i386
          -lblas_i386
```
- Compile the program typing “`gmake`” for optimized version and “`gmake debug=true`” for debugger version. If your computer system is not automatically recognized you will need to specify in addition either “`ht={system identification}`” on SUN and IBM systems, where “{system identification}” should be “`sun`” or “`ibm`”, respectively, or “`htype={system identification}`” on COMPAQ Alpha computers and PCs, where “{system identification}” has to be replaced by “`alpha`” or “`i386`”, respectively. For example, to get a debugging version on a SUN workstation you should type “`gmake debug=true ht=sun`”, and for an optimized version on an INTEL PC “`gmake htype=i386`” has to be typed.

2.5 How to run SCIATRAN

- If “`$VENDOR`”/“`$HOSTTYPE`” system variables are correctly set in your shell you can run SCIATRAN using a shell script “`run_scia`” which automatically determines your computer system, removes all output files from previous program run, and starts an appropriate executable. For debugger version just type “`run_scia debug`”. Otherwise you can run the program typing “`./SCIA_{COMPUTER SYSTEM}.exe`” or “`./SCIA_{COMPUTER SYSTEM}_DBG.exe`” for debugging version. Here, “{COMPUTER SYSTEM}” has the same meaning as described above, i.e., for example, to start the optimized version on a COMPAQ Alpha computer you need to type “`SCIA_ALPHA.exe`”.
- If the program run was successful you will see the following message at the end of the screen output:

```
***** RT calculations terminated successfully *****
***** Results are stored according to *****
***** ./DATA_OUT/output_map.inf *****

***** Normal termination *****
```

- All output data are stored in “`DATA_OUT`” subdirectory. See “`DATA_OUT/output_map.inf`” to find appropriate output files. Please note, “`DATA_OUT`” is a program working directory. Do not store any important files therein, they can be lost otherwise!

2.6 Control files

- `control.inp` - main control file.
- `control_geom.inp` - geometry settings.
- `control_ac.inp` - settings related to the accuracy of the radiative transfer modeling. Please, bear in the mind that an increased accuracy slows down the program and vice versa.
- `low_aer.inp`, `scia_aer.inp`, and `man_aer.inp` - control files containing aerosol parameters depending on aerosol parameterization selected in `control.inp`, only needed if aerosols are switched on in `control.inp`.
- `cloud.inp` - control file containing cloud parameters, only needed if clouds are switched on in `control.inp`.
- `xsections.inp` - control file containing information about cross sections, always needed.
- `esft.inp` - initialization of the esft computation scheme (does not need to be changed by users)
- `control_ret.inp` - control file containing information needed for running SCIATRAN in the retrieval mode.

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, “Do aerosols”) and subsequent lines of input parameters (for example: “F” for “false”). Only those lines containing the input parameters 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.

Chapter 3

Radiative transfer modeling with SCIATRAN

3.1 Type of the radiative transfer modeling

Appropriate control file: “control.inp”

Relevant control parameters: “RTM_TYPE”

Setting “RTM_TYPE” to “spher_scatt”, “pp_scatt”, or “ps_scatt”, the solar radiation scattered by the Earth’s atmosphere or 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 below, Sec. 3.2.

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.

3.2 Sphericity of the atmosphere

Appropriate control files: “control.inp”, “control_geom.inp”

Relevant control parameters: “RTM_TYPE”

This section is irrelevant if solar/lunar occultation mode is selected, i.e., “RTM_TYPE” parameter is set to “transmission”.

3.2.1 Plane-parallel atmosphere

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_scatt”. 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. The mode is not supported if “RTM-CORE” is set to “CDI” (automatically switched to pseudo-spherical mode).

Limitations:

- increasing errors for solar zenith angles larger than $\sim 75^\circ$;
- approximation is not valid for solar zenith angles larger than/equal to 90° ;
- increasing errors for line-of-sight angles larger than $\sim 20^\circ$ depending on solar zenith angle, wavelength, etc.;
- not appropriate for limb viewing geometry.

3.2.2 Pseudo-spherical atmosphere

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_scatt”. In this mode the radiative transfer equation is solved in the plane-parallel atmosphere whereas the source term (right hand side of the RTE) 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 to simulate measurements of the scattered solar radiation during the twilight in zenith or nadir viewing geometry. The pseudo-spherical mode is automatically switched on if “RTM-CORE” is set to “CDI” in the plane-parallel mode (“RTM_TYPE” set to “pp_scatt”).

Limitations:

- increasing errors for solar zenith angles larger than $\sim 92^\circ$;
- increasing errors for line-of-sight angles larger than $\sim 30^\circ$ depending on solar zenith angle, wavelength, etc.;
- not appropriate for limb viewing geometry.

3.2.3 Spherical atmosphere

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_scatt”. 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. 3.3.

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” 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.

Limitations:

- the multiple scattering is set to zero for solar zenith angles large than 98° ;
- in “CDI” mode only Henyey-Greenstein phase function for aerosols is available, no delta-M/delta-fit approximation is possible;
- clouds can only be considered in “DOM” mode;
- weighting functions for pressure, temperature, Rayleigh and aerosol scattering, as well as average number of photon scattering events (ANPS) are only available in “DOM” mode.

3.2.4 Curvature of the atmosphere and the refraction

Appropriate control file: “control_geom.inp”

Relevant control parameters: “Do 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 “Do refractive geometry” to “t”.

Limitations:

- No wavelength dependence of the refraction index is implemented.

3.3 Radiative transfer codes

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 3.1).

3.3.1 Fully featured solvers (“`CDI`” and “`DOM`”)

Appropriate control file: “`control.inp`”

Relevant control parameters: “`RTM-CORE`”

Setting the “`RTM-CORE`” control parameter to “`CDI`”, the CDI/CDIPI radiative transfer model [37, 38] 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_scatter`” or “`spher_scatter`”, 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_scatter`”) or for a spherical (“`RTM_TYPE`” is set to “`spher_scatter`”) 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. 3.2.3, 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 in “`CDI`” mode:

- plane-parallel mode is 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 Sec. 3.6.3
- weighting functions are available for trace gas concentrations only.

Setting the “RTM-CORE” control parameter to “DOM”, the discrete ordinate model is selected. This solver can be used in any sphericity mode (any setting of “RTM_TYPE”). In the plane-parallel and pseudo-spherical modes, the radiative transfer equation is solved for selected line-of-sights only, employing the discrete ordinate method and Fourier series expansion. The weighting functions are obtained using the adjoint solution method. In the spherical mode, the radiance is calculated similar to the “CDI” mode performing an integration along the line-of-sight and using the pseudo-spherical radiation field to estimate the multiple scattering contribution, whereas the weighting functions are calculated using the adjoint approach.

Limitations in “DOM” mode:

- 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. 3.12.4;
- the bidirectional reflectance distribution function (BRDF) is not available, see Sec. 3.13;

3.3.2 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” a new effective approximation for the radiative transfer modeling in a presence of clouds based on an asymptotic formula [21] is used in calculations. This mode is extremely fast, however, it can not be used in a cloud-free atmosphere, i.e., “Clouds present” parameter must be set to “t”. This mode can be used in the plane-parallel atmosphere only (“RTM_TYPE” is set to “pp_scat”), see Section 3.2.

Limitations:

- Only one cloud layer is supported, i.e., “Number of cloud layers” must be set to “1” (see Section 3.18.1)
- 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 3.18.2-3.18.4)

3.4 What do you intend to calculate?

Appropriate control file: “control.inp”

Relevant control parameters: “RTM Mode”

By means of “RTM Mode” control parameter user can switch between 11 major program modes depending on what is intended to be calculated. The program modes available in SCIATRAN 2.2 are described in details below.

3.4.1 Intensity/radiance (“int”)

Relevant control parameters: “RTM Mode”, “Absolute radiance”, “RTM-CORE”, “Angle interpolation approach”

Setting “RTM Mode” parameter to “int”, the intensity of radiation field is calculated. The output units depend on the the setting of “Absolute radiance” parameter (see Section 3.7). The intensity of radiation will be referred to as the intensity if the solar irradiance at the top of atmosphere is set to π and as the radiance otherwise. The expression irradiance will be used for the extraterrestrial radiant flux crossing an unit surface perpendicular to the axis of the radiation beam at the top of atmosphere.

In the discrete ordinate mode (“RTM-CORE” control parameter is set to “DOM”) user can choose between two methods to obtain the outgoing radiation traveling in the user-defined direction from the general solution of the radiative transfer equation. This is done using the “Angle interpolation approach” control parameter in “control.ac.inp” file. The standard setting is the source function integration approach which is selected setting the “Angle interpolation approach” control parameter to “sfi”. In this approach the outgoing radiation is calculated using the entire radiative field resulted from the solution of the radiative transfer equation. If the outgoing intensity has to be simulated for a large number of solar zenith angles ($\gtrsim 50$) the radiative transfer modeling can be speeded up using the adjoint solution integration approach which is selected setting the “Angle interpolation approach” control parameter to “asi”. In this case the resulting outgoing radiation is calculated employing the adjoint solution. Please note, the speed up takes place only in the intensity simulation mode, i.e., if the ‘RTM Mode’ control parameter is set to “int”. Details on the integration approaches can be found in [40].

3.4.2 Weighting functions (“wf”)

Relevant control parameters: “RTM Mode”, “RTM.TYPE”, “Absolute radiance”, “RTM-CORE”, “Trace gas selection - weighting functions”, “Other parameters - weighting functions”, “WF normalization”, “Absolute or relative WF”, “WF integration mode”

Setting “RTM Mode” parameter to “wf”, weighting functions and intensity/radiance are calculated. The intensity/radiance 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 “Absolute radiance” parameter (see Section 3.7). Parameters which the weighing function will be calculated for are selected by setting appropriate flags in “Trace gas selection - weighting functions” and “Other parameters - weighting functions” control lines to “t”. Most of the weighting functions can be used either in the relative or in the absolute representation setting “Absolute or relative WF” parameter to “rel” or “abs”, respectively. The relative weighting functions are multiplied by the vertical distributions 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. However, some weighting functions are not affected by this setting, for example, the weighting functions for the temperature, surface elevation, and tangent height as well as the average number of photon scattering events are always absolute, whereas the pressure weighting function remains always relative. Additionally, an integration type of the weighting function can be controlled setting “WF integration

mode” parameter to “**analytic**”, “**numeric**”, or “**nointegr**”. Depending on this setting weighting functions can be integrated over each layer analytically, numerically or calculated without an integration, respectively. Furthermore, in “**DOM**” 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.

Limitations:

- In the solar/lunar occultation mode (parameter “**RTM_TYPE**” set to “**transmission**”) only trace gas weighting functions can be calculated (controlled by the “**Trace gas selection - weighting functions**” parameter line). Any settings in “**Other parameters - weighting functions**” control line 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 “**Other parameters - weighting functions**” control line 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.inp**” file.

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 Sections 3.10, 3.17, and 3.18 to learn how to switch forward model parameters on/off).

3.4.3 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 3.12.4) for the selected gas are calculated.

3.4.4 Fluxes (“flux”)

Relevant control parameters: “RTM Mode”, “RTM_TYPE”, “Absolute radiance”, “Lower and upper boundary of flux results”

Setting “RTM Mode” parameter to “flux” the following fluxes are calculated:

- actinic flux ;
- upwelling and downwelling diffuse fluxes ;
- upwelling and downwelling total fluxes.

Furthermore, the direct solar radiance at each height level is computed. The output units are controlled by “Absolute radiance” parameter (see Section 3.7).

The fluxes and the direct solar radiance are calculated at all altitude levels defined by the standard altitude grid (see Section 3.5) and all solar zenith angles specified in “Solar zenith angles” control field (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). 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 “Absolute radiance” parameter is set to “t”, solar irradiance is written out as well.

Limitations:

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

3.4.5 Spherical albedo (“spher_alb”)

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

Setting “RTM Mode” parameter to “spher_alb” the diffuse reflected and transmitted spherical albedo are calculated.

The spherical albedo is calculated at all altitude levels defined by the standard altitude grid (see Section 3.5) 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). 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. The only relevant parameter for this mode is the number of solar zenith angles which is used by the program for the integration of the intensity over the solar zenith angles. The choice of the solar zenith angles is done automatically.

Limitation:

- the spherical albedo 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”).

3.4.6 Vertical optical depth (“vod”)

Relevant control parameters: “RTM Mode”, “RTM_TYPE”, “RTM-CORE”, “Trace gas selection - forward model”

Setting “RTM Mode” control parameter to “vod” the vertical optical depths for atmospheric trace gases selected in “Trace gas selection - forward model” (see Section 3.10) are calculated. If “RTM-CORE” is set to “DOM” (see Section 3.3), the vertical optical depths for Rayleigh scattering, aerosol scattering and absorption, cloud scattering and absorption, as well as total optical depth are calculated additionally.

Limitations:

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

3.4.7 Rotational Raman scattering (“raman”)

Not available in SCIATRAN 2.x

3.4.8 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.

3.4.9 Weighting functions by numerical perturbations (“num_pert”)

Relevant control parameters: “RTM Mode”, “Lower and upper boundary for WF calculation”

Setting “RTM Mode” control parameter to “num_pert” allows some weighting functions to be calculated using the numerical perturbation method. The altitude range to calculate the numerical weighting functions is defined by the “Lower and upper boundary for WF calculation” control parameter.

This mode is intended for developing purposes only and should not be invoked by ordinary users.

3.5 Altitude grid

Appropriate control files “control.inp”

Relevant control parameters: “Altitude grid information”, “Height above sea level”, “Path to altitude grid file”, “Weighting parameter”

In “Altitude grid information” input field an altitude grid for radiative transfer model is to be specified. The input line contains the number of levels in the altitude grid and the name of the file containing the altitude grid. The path to this file has to be specified in “Path to altitude grid file” input line. The values in the altitude grid file should be arranged as a column and must be monotonously increasing or decreasing. Only the first input line below the keyword is relevant. 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.

In the CDI/CDIPI radiative transfer model (“RTM-CORE” is set to “CDI”, see Section 3.3) the optical properties of the atmosphere are defined at the altitude levels corresponding to the nodes of the altitude grid and interpolated between the levels, whereas in the Discrete Ordinate method (“RTM-CORE” is set to “DOM”) the optical properties of altitude layers are dealt with. Based on the optical properties specified for the altitude levels, the optical properties of the atmospheric layers are assigned using the “Weighting parameter” input line controlling how the optical parameters in each homogeneous layer are weighted. If “Weighting parameter” is set to “0” the layer is supposed to have optical properties specified at its lower boundary, if “Weighting parameter” is set to “1” the layer is supposed to have optical properties specified at its upper boundary. Default value is “0.5” resulting in averaging of optical purposes at lower and upper boundaries of each layer.

3.6 Accuracy of the radiative transfer modeling

Appropriate control file: “control_ac.inp”

3.6.1 Scattering modes

Relevant control parameters: “Scattering mode”, “SS/MS wavelength boundary”

Parameter “Scattering mode” allow user to reduce the computation time switching off the multiple scattering contribution to radiance and/or weighting functions. Please note, if the multiple scattering contribution is turned off no surface reflection is considered as well. The following modes are implemented:

- “ms” - fully multiple scattering treatment (default mode);
- “ss” - single scattering mode, both intensity/radiance 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.

Limitation:

- The discrete ordinate solver (“**RTM-CORE**” parameter is set to “**DOM**”, see Section 3.3) supports only the fully multiple scattering mode (“**Scattering mode**” parameter can only be set to “**ms**”).

A boundary wavelength in nm used to switch automatically between single scattering and multiple scattering modes (“**ms_ss**”, “**wf_ms_ss**”, and “**sm_wf_ss**” settings of “**Scattering mode**” parameter) is set in “**SS/MS wavelength boundary**” input field.

3.6.2 Sub-layers

Relevant control parameters: “**The number of fine grid layers**”, “**Fine grid start**”, “**Fine grid tangent**”, “**Fine grid height**”, “**The layering of line-of-sight**”

The accuracy of the radiative transfer calculations in a presence of a strong vertical inhomogeneity can be increased dividing the altitude layers as defined by the standard 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 three 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 (if 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.

Limitations:

- These settings have no effect in a plane-parallel atmosphere (“RTM_TYPE” is set to “pp_scat”, see Section 3.1).
- If the discrete ordinate solver (“RTM-CORE” is set to “DOM”, see Section 3.3) 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”), an additional gridding 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 gridding 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, from 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 extension 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. 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 3.4.

3.6.3 Adaptive grid in the Discrete Ordinates Method

Relevant control parameters: “Adaptive grid”, “Homogeneity criteria”

If the Discrete Ordinate method is employed (“RTM-CORE” is set to “DOM”, see Section 3.3) the radiative transfer calculations can be substantially accelerated without any noticeable loss of the accuracy setting the “Adaptive grid” to “t”. In this mode, the vertical inhomogeneity of the atmosphere is analyzed 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. The criterion to decide whether the single scattering albedos of two 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%.

3.6.4 Fourier series/Legendre moments development

Relevant control parameters: “Single scattering correction”, “Azimuth series flag”, “Do only 0th harmonic for near nadir”, “Near nadir definition [deg]”, “Accuracy criterion”, “Number of streams”, “Number of Legendre moments”

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**” (see Section 3.3).

The single scattering correction activated by setting the “**Single scattering correction**” control parameter to “**t**” is done by subtracting from the total scattered radiance 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:

- only satellite observation mode (see Section 3.8.1) is supported, no user-defined output altitude can be set (see Section 3.8.2);
- only one solar zenith angle can be selected (see Section 3.8.1);
- only “user” type of phase function is supported for clouds (see Section 3.18).

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. Otherwise, only zeroth harmonic will be taken into account.

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 both satellite and ground based observation modes.

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.

The input parameter “**Number of streams**” controls the number of Gaussian nodes used to discretize the angular integrals in the radiative transfer equation. The selected value should be greater than $0.43 \times (\text{“Number of Legendre moments”} - 1)$.

3.7 Irradiance

Appropriate control file: “**control.inp**”

Relevant control parameters: “**Absolute radiance**”, “**Filename user provided solar spectrum**”

If “**Absolute radiance**” parameter is set to “**t**” the output spectra will be converted to absolute units multiplying by the solar irradiance spectrum provided in “**Filename user provided solar spectrum**” control line. The output units are determined by the units of the irradiance spectrum supplied by user.

If “**Absolute radiance**” parameter is set to “**f**” the solar irradiance is supposed to be equal π at all wavelengths.

3.8 Observation geometry

Appropriate control file: “control_geom.inp”

3.8.1 Instrument viewing direction

Relevant control parameters: “Do satellite”, “Angle selection mode”, “The number of solar zenith angles”, “The number of viewing angles”, “The number of azimuth angles”, “Solar zenith angles”, “Field of view integration”, “Field of view size”

“Do satellite” 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 the “satellite observation mode” is appropriate and “Do satellite” parameter should be set to “t”. In opposite, for ground based measurements as well as for upward looking air- and balloon-borne instruments the “ground based observation mode” is appropriate and “Do satellite” parameter should be set to “f”.

“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”, “The number of viewing angles”, and “The number of 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).

Limitations:

- if “RTM-CORE” parameter is set to “ASYMP” (see Section 3.3) each of “The number of solar zenith angles”, “The number of viewing angles”, and “The number of azimuth angles” parameters must be set to “1”;

- if “Single scattering correction” parameter is set to “t” (see Section 3.6.4) “The number of solar zenith angles” parameter must be set to “1”.

The control parameter “Solar zenith angles” defines the values of the local solar zenith angle at observer position in deg. 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.

Limitations:

- in plane-parallel mode (see Section 3.2.1) errors are increasing for solar zenith angles larger than $\sim 75^\circ$
- in pseudo-spherical mode (see Section 3.2.2) errors are increasing for solar zenith angles larger than $\sim 92^\circ$
- in spherical mode (see Section 3.2.3) multiple scattering contribution at solar zenith angles larger than 98° is set to zero.

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 3.2) and larger than top of the atmosphere (see Section 3.5);
- “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 (“Do satellite” is set to “t”) and “zenith” in ground based observation mode (“Do satellite” is set to “f”);
- “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 number of viewing angles” parameter. This mode is only available if “Angle selection mode” is set to “all”.

The control parameter “Viewing angles” defines the values for line-of-sight angle (also referenced as viewing angle or zenith angle) 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 3.2) .
- in non-spherical mode errors may be increasing for viewing angles larger than $\sim 30^\circ$ depending on solar zenith angle, viewing direction, observer position, wavelength, etc.

The control parameter “Azimuth angles” defines the values for the relative azimuth angle 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.

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.

Limitations:

- In the discrete ordinate mode (“RTM-CORE” parameter is set to “DOM”, see Section 3.3) the field of view integration is only supported for a spherical atmosphere (see Section 3.2).

3.8.2 Observer position

Relevant control parameters: “Flag for user-defined output altitude”, “User-defined output altitude”

By default, the observer position is defined by “Do satellite” flag. The instrument is supposed to be located at the top of the atmosphere in the satellite observation mode (“Do satellite” is set to “t”) and at the surface in the ground based observation mode (“Do satellite” is set to “f”). Setting “Flag for user-defined output altitude” to “t” an instrument position in the atmosphere or above the atmosphere can be specified by user. The corresponding value is defined setting parameter “User-defined output altitude” to the desired altitude in km. Selected altitude must not be below the surface.

Limitation:

- user-defined altitude can not be set if “Single scattering correction” parameter is set to “t” (see Section 3.6.4)

3.9 Spectral intervals

Appropriate control file: “control.inp”

Relevant control parameters: “Wavelength segment info”

Generally, any spectral interval between 175.44 nm and 2400 nm can be selected. However, aerosols can only be switched on at wavelengths longer than 240 nm (see Section 3.17). 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 line in “Wavelength segment info” control field. The input spectral information is then read by the program from lines below starting from the second line in “Wavelength 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 in nm, number of required wavelengths, and stepsize in nm, respectively;
- “2” - the values from the second to the fourth in the line will be interpreted as start wavelength in nm, end wavelength in nm, and stepsize in nm, respectively.

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

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

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. 3.4.8) 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 “Wavelength segment info” control field.

3.10 Atmospheric trace gases - spectral information

Appropriate control file: “control.inp”

Relevant control parameters: “Trace gas selection - forward model”

The following atmospheric trace gases implemented at present: O₃, NO₂, ClO, OClO, BrO, HCHO, SO₂, NO₃, O₄, O₂, H₂O, CO₂, CO, CH₄, and N₂O

Due to a different treatment of spectral information one should distinguish between so-called “line-absorbers”, such as H₂O, CO₂, CO, CH₄, and N₂O, which feature complex absorption bands strongly dependent on pressure and temperature and ordinary “continuum-absorbers”, such as O₃, NO₂, ClO, OClO, BrO, HCHO, SO₂, NO₃, O₄. A special treatment is needed for O₂ which is considered as a “continuum-absorber” in UV spectral region and as a “line-absorber” in Vis-NIR spectral region. A contribution of a particular trace gas into the total absorption can be switched on or off setting an appropriate flag in “Trace gas selection - forward model” control line to “t” or “f”, respectively.

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.

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 [1] (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.

Cross sections need not to be specified for trace gases switched off in “Trace gas selection - forward model” control line.

Two separate inputs are needed to describe O₂ 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. At present, temperature parameterization is available in Schumann-Runge absorption band only.

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. A type of temperature

parameterization can be selected between GOME FM [8, 9] and Bass-Paur [28] 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. There is no temperature parameterization available below 240 nm. A discontinuity may occur at joint points.

3.10.2 Treatment of “line-absorbers”

Appropriate control file: “control.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 [32]. The following program modes selected by setting “Line absorber treatment” parameter to a desired keyword are implemented in order to accurately consider “line-absorbers”:

- “lb1” - 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 [5, 6, 7] 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 “Trace gas selection - forward model” control line.

Due to a strong spectral variability of the absorption features of “line-absorbers” a quite small wavelength step should be selected in “Wavelength 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 obtained 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” 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”

Relevant control parameters: “Spectroscopic line parameter filename”, “Isotopic line parameter filename”, “Line absorber treatment”, “Line wing cut-off wavenumber”

Line-by-line mode is selected if “Line absorber treatment” parameter is set to “lbl”. In this mode two additional paths to HITRAN database files need to be set in input fields “Spectroscopic line parameter filename” and “Isotopic line parameter filename”. The filenames 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”, “esft.inp”

Relevant control parameters: “Path to ESFT data base”, “Line absorber treatment”, “Do esft anti correlation”, “Path to ESFT data base”

ESFT mode is selected if “Line absorber treatment” parameter is set to “esft”. In this mode an additional path to the ESFT data base should be specified in “Path to ESFT data base” input field.

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.

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

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 ₂ O, O ₂
6	1070 - 1800	0.2	H ₂ O, CO ₂ , O ₂ , CH ₄
7	1920 - 2060	0.025	CO ₂ , H ₂ O
8	2230 - 2340	0.025	CH ₄ , CO, H ₂ O, N ₂ O

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`”

Relevant control parameters: “`Do convolution`”, “`Convolution for line absorber only`”, “`Slit function type`”, “`Slit function HWHM`”, “`Slit function wing cut-off`”, “`Internal wavelength step`”

“`Do convolution`” parameter is used to control if convolution is 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 “`Wavelength segment info`” input field (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 “`Internal wavelength step`” is used. Please note that you need to set quite small wavelength step to get a reasonable accuracy in line-by-line mode (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 following parameters defining the shape of the instrument slit function need to be specified:

- “Slit function type” - at present only Gaussian slit function is supported;
- “Slit function HWHM” - slit function half width at half maximum in nm, needs to be specified for each spectral interval selected in “Wavelength 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.

3.12 Atmospheric trace gases - vertical distributions

Appropriate control file: “control.inp”

3.12.1 General

Relevant control parameters: “Do profiles akima interpolation”, “Standard profile scenario file name”, “Standard profile scenario for line absorbers”

Parameter “Standard profile scenario file name” defines the name of the file containing vertical distributions of “continuum-absorbers” (O₃, NO₂, SO₂, ClO, BrO, NO₃, HCHO, and OCIO), see Section 3.10, as well as vertical profiles of pressure and temperature. The vertical distribution for O₄ is calculated from the air density profile. By default, a climatological data base obtained using a 2D chemo-dynamical model developed at MPI Mainz [3] 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. If the top of atmosphere height is set to a value higher than 60 km (see Section 3.5) 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. The corresponding filenames usually have the following structure: “mon{xx}lat{yy}{z}.mpi”, 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).

Alternatively, either McLinden climatology (C. McLinden, Meteorological Service of Canada, privat communication) containing monthly and latitudinal dependent vertical distributions of O₃, NO₂, BrO, and OCIO volume mixing ratios, as well as pressure and temperature in the altitude region between 0 and 100 km or US Standard atmosphere [27] containing zonally and seasonally averaged vertical distributions of O₃, NO₂, SO₂, and ClO volume mixing ratios, as

well as pressure and temperature in the altitude region between 0 and 120 km can be used. The filenames appropriate to McLinden climatology have the same structure as for MPI climatology files: “`mon{xx}lat{yy}{z}.mc1`” and the US Standard atmosphere is represented by “`uss76.dat`” file. Atmospheric trace gases switched on in “`Trace gas selection - forward model`” 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.

The control parameter “`Standard profile scenario for line absorbers`” defines the name of the file containing vertical distributions of “line-absorbers” (O_2 , H_2O , CO_2 , N_2O , CO , CH_4), see Section 3.10. The only 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”. Corresponding profiles are stored in “`usstandard.dat`” file.

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 [1] (setting “`t`”) will be employed instead.

3.12.2 Replacements

Relevant control parameters: “`Do P and T from standard profile file`”, “`Pressure and temperature file name`”, “`Trace gas replacement profiles`”

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.

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 O₃ and NO₂ will be replaced, no replacement will be done for BrO. The first data column of “conc_const.o3” is supposed to contain the altitude grid appropriate to the replacement profile of O₃ contained in the second data column. The replacement profile is expected to be supplied as a vertical distribution of O₃ 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 NO₂ contained in the sixth data column. The replacement profile is expected to be supplied as a vertical distribution of NO₂ volume mixing ratio in ppmv.

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 O₃ and temperature read from an ozone climatology, see Section 3.12.3, are replaced as well.

3.12.3 Ozone climatologies

Relevant control parameters: “Ozone climatology”, “Scale climatological profile”, “Ozone total column”, “Path to ozone climatology”

Ozone climatologies can be used setting the “Ozone climatology” control parameter to any supported value other than “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 of Environmental Physics/Institute of Remote Sensing (University of Bremen) based on ozonesonde and satellite data [23]. 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 [45]. 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 [14]. 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 Reading¹ 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 3.15.
- 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 3.15.
- 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.

3.12.4 Photochemistry

Relevant control parameters: “Photochemical calculations”, “Number of photochemically active species”, “Trace gas selection - photochemistry”, “Tropopause height”, “Use constant profile”, “Solar zenith angle for constant profile”, “Altitude grids for

¹<http://badc.nerc.ac.uk/data/ugamp-o3-climatology/>

photochemically active species”, “Profiles for photochemically active species”, “Replace tropospheric concentrations”

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) 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 3.3).

3.13 Surface

Appropriate control files: “control.inp”

Relevant control parameters: “Albedo”, “Do spectral albedo from data base”, “Spectral albedo filename”, “BRDF flag”, “Surface type”, “BRDF spectral range”

A constant albedo for a Lambertian surface is set in “Albedo” input line. If “Do spectral albedo from data base” parameter is set to “t”, a wavelength dependent albedo from the spectral database specified in “Spectral albedo filename” is used instead of a constant value. 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

If “RTM-CORE” is set to “CDI” (see Section 3.3) a non-Lambertian surface can be modeled using an appropriate parameterization for the bidirectional reflectance distribution function (BRDF) [25, 29, 12, 11]. This is done setting “BRDF flag” parameter to “t”. A desired surface type is selected in “Surface type” control line. The following settings are supported: “spruce”, “sparse erectophile”, “tropical forest”, “plowed field”, “grasses”, “broad leaf crops”, “Savannah”, “leaf forest”, “Conifers”, “hardwood forest winter”, “loam soil”, “irrigated wheat”, “dark”, “bright”, “snow”, “ocean”.

For most surface types two different parameterizations for UV and near-IR spectral ranges are available. A desired spectral range is selected setting “BRDF spectral range” parameter to “UV” or “IR”.

3.14 Specification by geolocation

Appropriate control files: “control.inp”

Relevant control parameters: “Do specification by geolocation”, “Do profile latitude

interpolation”, “Stop after generating CLIMATOLOGY.OUT”, “Path to climatology data base”

If “Do specification by geolocation” is set to “t” some input settings will be automatically changed according to the selected date and geolocation (see Section 3.15). An appropriate setting of “Path to climatology data base” control parameter is required. The following parameters are affected:

- File specified in “Standard profile scenario file name” control line containing vertical distributions of “continuum-absorbers” will be replaced by an appropriate file from the MPI database, see Section 3.12.1. Replacement profiles (see Section 3.12.2) and climatological ozone profiles (see Section 3.12.3) are not affected.
- Surface elevation defined by “Height above sea level” parameter (see Section 3.5).
- Surface type used to select an appropriate spectral albedo database (see Section 3.13). If “Do spectral albedo from data base” is set to “f” the constant albedo specified in “Albedo” input line will be replaced by a value at 760 nm from the appropriate spectral database.

If “Stop after generating CLIMATOLOGY.OUT” control parameter is set to “t” the program will stop after writing settings to be changed according to the specified date and geolocation into the “CLIMATOLOGY.OUT” file (see Section 3.20).

The input parameter “Do profile latitude interpolation” controls if a latitudinal interpolation of trace gas vertical distributions from the MPI data base will be performed. If “Do profile latitude interpolation” parameter is set to “f” vertical distributions of “continuum-absorbers” corresponding to the latitude closest to the specified geolocation will be selected from the MPI data base.

3.15 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” is set to any supported value other than “NONE” (see Section 3.12.3) or to select appropriate vertical distributions of atmospheric trace gases from MPI climatology, appropriate surface elevation, and an appropriate surface type if specification by geolocation is done (see Section 3.14).

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.

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.

3.16 Rayleigh scattering settings

Appropriate control files: “control.inp”

Relevant control parameters: “Rayleigh scattering index”, “Rayleigh depolarisation value”, “Rayleigh depolarisation wavelength dependent?”, “Rayleigh depolarisation filename”

By means of “Rayleigh scattering index” parameters different formulas to calculate Rayleigh scattering coefficient can be selected. This parameter should be set to “7” (corresponds to the scattering coefficient given by D.R. Bates) unless you explicitly want to use any other formula. Setting “Rayleigh depolarisation wavelength dependent?” parameter to “t”, wavelength dependent values for Rayleigh depolarisation factor will be read from the file specified in “Rayleigh depolarisation filename” input line. Otherwise, the Rayleigh depolarisation factor will be set to a constant value specified in “Rayleigh depolarisation value” control line.

Although the Rayleigh scattering can not be switched off, its contribution can be changed scaling the Rayleigh scattering coefficient. The scaling factor is determined by the “Rayleigh scattering depletion” input line and is the same for all wavelengths. If the first value in this control line is set to “t”, the Rayleigh scattering coefficient will be divided by the second value specified in the input field.

3.17 Aerosols

Appropriate control files: “control.inp”, “low_aer.inp”, “scia_aer.inp”, “man_aer.inp”

Relevant control parameters: “Do aerosols”, “Aerosol parameterization type”, “Aerosol phase function index”, “Aerosol delta-M approximation”, “Truncation index for delta-M approximation”, “Path to aerosol data base”, “Aerosol scaling parameter”

Scattering and absorption by aerosols is considered in the radiative transfer calculations if “Do aerosols” flag is set to “t”.

Changing the setting of the “Aerosol parameterization type” control parameter between “st”, “lt”, and “mn” the SCIATRAN [15, 18], the LOWTRAN [41, 19], or the user-defined aerosol parameterization, respectively, is selected. By default, the LOWTRAN aerosol parameterization is used in SCIATRAN 2.2. Parameterization specific aerosol settings which are not the subject of this User’s Guide can be found in “scia_aer.inp” and “low_aer.inp” control files for SCIATRAN and LOWTRAN parameterizations, respectively. The SCIATRAN aerosol parameterization requires additionally the path to the aerosol database to be specified in the “Path to aerosol data base” input line. If the user-defined aerosol parameterization is selected, wavelength independent vertical profiles of the aerosol extinction and absorption coefficients as well as

a parameterization for the aerosol phase function can be supplied manually in the “`man_aer.inp`” control file. Depending on the setting of the “`Aerosol phase function parameterization`” control parameter, the aerosol scattering phase function is defined as follows:

- “`HG_asym`” - the aerosol phase function is defined by the asymmetry factor according to the Henyey-Greenstein parameterization. The asymmetry factor can be specified as a function of the altitude in the “`Asymmetry factor`” control field. The format of the input field is described below.
- “`Num_sca`” - the aerosol phase function is defined numerically as a function of the scattering angle. The parameterization has to be supplied in a file which is formatted as follows. The header lines must be separated from the data block by a line containing “`>`” as the first character. The first input line below this separation line has to contain the number of scattering angles which the phase function is defined for. The subsequent data block contain scattering angles in degrees in the first column and appropriate values of the phase function in the second column. The parameterization can be specified at each altitude level independently in the “`Filenames for aerosol phase function`” input field specifying appropriate filenames. The detailed description of the input field format is given below.
- “`LSE_coeff`” - the aerosol phase function is represented by the Legendre series expansion coefficients. The parameterization has to be supplied in a file which is formatted as follows. The header lines must be separated from the data block by a line containing “`>`” as the first character. The first input line below this separation line has to contain the number of Legendre series expansion coefficients supplied in the file. The subsequent data block contain the expansion coefficients in the second column. The first column in the data block is not used. The parameterization can be specified at each altitude level independently in the “`Filenames for aerosol phase function`” input field specifying appropriate filenames. The detailed description of the input field format is given below.

Limitation:

- “`Num_sca`” and “`LSE_coeff`” parameterizations can be used in “`DOM`” mode only (see Section 3.3).

The aerosol extinction and scattering coefficients are supplied in km^{-1} using the “`Extinction coefficient`” and “`Absorption coefficient`” input fields, respectively. The format of both input fields is the same as for phase function parameterizations.

All input fields are marked by a keyword describing the parameter to be read. Each keyword is followed by an integer value specifying the number of the altitude levels where the vertical profile of the corresponding aerosol parameter will be defined. Thus, this parameter defines the number of the subsequent lines in the input field which will be read by the program. All lines below will be ignored. Minimum two levels are required. The lines starting from the second after the keyword, i.e., immediately below the number of the altitude levels, contain the altitude in `km` as the first entry and the parameter value or the parameter filename as the second entry. The vertical profiles of all aerosol parameters will be linearly interpolated between the input altitude levels and extrapolated with zero above the highest and below the lowest input level.

The input parameter “**Aerosol phase function index**” controlling the type of the aerosol phase function can be set to “1” or “2” selecting either Mie or Henyey-Greenstein type of the phase function, respectively. The Mie phase function type can only be selected if the SCIATRAN aerosol parameterization is used. This setting has no effect if the user-defined aerosol parameterization is selected (“**Aerosol parameterization type**” control parameter is set to “mn”).

Changing the setting of “**Aerosol delta-M approximation**” control parameter between “D-M”, “D-F”, and “all” user can switch between Delta-M approximation [46], Delta-Fit approach [17], or use all available Legendre moments (as defined by “**Number of Legendre moments parameter**”, see Section 3.6.4), respectively. A desired number of phase function moments which will be used to approximate the aerosol phase function is controlled by “**Truncation index for delta-M approximation**” parameter which must be smaller than the value defined by “**Number of Legendre moments**” parameter. Settings of “**Aerosol delta-M approximation**” and “**Truncation index for delta-M approximation**” input parameters have no effect if the “**RTM-CORE**” control parameter is set to “CDI” (see Section 3.3), as well as in the solar/lunar occultation mode (see Section 3.1).

The specified aerosol loading can be also 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 default value is “1.0” which retain all previously selected aerosol parameters unchanged.

Limitations:

- Aerosols are not supported at wavelengths shorter than 240 nm;
- No wavelength dependence of the aerosol characteristics can be accounted for if the user-defined parameterization is selected;
- Mie phase function is only supported in the discrete ordinate mode (“**RTM-CORE**” control parameter is set to “DOM”, see Section 3.3) using the SCIATRAN aerosol parameterization. The maximal number of the phase function moments is limited to 50.

3.18 Clouds

Appropriate control files: “control.inp”, “cloud.inp”

Relevant control parameters: “**Clouds present?**”

All settings discussed in this section have only an effect if “**Clouds present?**” parameter in “control.inp” is set to “t”. Clouds are not supported if “**RTM-CORE**” is set to “CDI” (see Section 3.3).

Talking about cloud parameters the following terminology needs to be introduced:

- **water/ice cloud** - cloud consisting of either water droplets or ice crystals;
- **mixed cloud** - cloud consisting of a mixture of water droplets and ice crystals;

- **cloud layer** - the part of the atmosphere between a cloud bottom and cloud top;
- **vertically homogeneous cloud** - all optical parameters of the cloud are constant within a cloud layer;
- **vertically inhomogeneous cloud** - optical parameters of the cloud are altitude dependent within a cloud layer;
- **integral parameters** - parameters describing integral properties of a cloud layer, such as optical thickness (τ), liquid water path (LWP), ice water path (IWP);
- **geometrical parameters** - cloud top height (h_t), cloud bottom height (h_b), and cloud geometrical thickness ($h_t - h_b$).

3.18.1 General

Appropriate control file: “cloud.inp”

Relevant control parameters: “Path to cloud data bases”, “Number of cloud layers”, “Cloud layer base and top”, “Cloud sub-layers number”, “Thermodynamic state”, “Delta-M or Delta-Fit”, “Delta-m truncation for cloud layers”, “Cloud particle profile input file”

A path to the cloud database is to be set in “Path to cloud data bases” input line.

The control parameter “Number of cloud layers” defines the number of cloud layers to be considered in the radiative transfer model. The case with the number of cloud layers greater than 1 corresponds to the multilayered cloud system.

Values for the base and the top altitudes should be defined for each cloud layer in “Cloud layer base and top”. In a case of a multilayered cloud system, cloud layers have to be arranged in an increasing order, i.e., from the bottom to the top of the atmosphere. 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 layer-specific cloud parameters.

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 can be between 2 and 50.

Changing the setting of “Delta-M or Delta-Fit” control parameter between “D-M” and “D-F” user can switch between Delta-M approximation [46] and Delta-Fit approach [17], respectively. This setting is valid for all cloud layers, only one input line is required. A desired number of phase function moments which will be used to approximate the full phase function within a cloud layer is controlled by “Delta-m truncation for cloud layers” parameter. This parameter has to be set for each cloud layer independently.

In order to describe a particular cloud layer, the following optical parameters have to be defined: phase function, extinction coefficient, σ_e , and scattering coefficient, σ_s . Generally, there are two ways to initialize these parameters:

- use a pre-calculated data base containing extinction coefficients, single scattering albedo, and phase function moments for 9 standard cloud models characterized by the effective radius of water droplets (4, 6, 8, 10, 12, 14, 16, 18, and 20 μm) covering a spectral range between 0.2 and 5 μm ;
- supply a user-defined file containing σ_e , σ_s , and phase function moments, no wavelength dependence can be considered.

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 can be set to “**water**”, “**ice**”, or “**mixed**” defining water clouds, ice clouds, or mixed clouds, respectively. Parameter settings appropriate to different thermodynamic states of a particular cloud layer are described in Sections 3.18.2-3.18.4 in detail. All parameters defining a cloud in a particular thermodynamic state discussed below must be set for each cloud layer independently.

In particular 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 to “`../data/clouds/cld_prof.hom`” or “`../data/clouds/cld_prof.vin`” containing examples for a vertically homogeneous and a vertically inhomogeneous cloud, respectively.

The general structure of these files is as follows:

- all lines before the line containing symbol “>” are treated as comment lines;
- the first column contains the dimensionless height from the cloud top to the cloud bottom: $(z_{top} - z)/(z_{top} - z_{base})$;
- the content of the second column depends on the setting in the “**Type of input integral parameter**” control field. This column is not used if the “**Thermodynamic state**” control parameter is set to “**ice**”;
- 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. This column is not used if the “**Thermodynamic state**” control parameter is set to “**water**”;
- the fifth column contains the profile of the ice crystal effective radius [μm].

Limitations:

- if the thermodynamical state of any cloud layer is set to “**mixed**”, the same thermodynamical state has to be selected for other layers;
- if the “**Type of input integral parameter**” control parameter is set to “**TAU**” (see below) in one water or ice cloud layer, it must be the same for any other layer;
- phase function is constant within a cloud layer but can be different for different cloud layers.

3.18.2 Water clouds

Appropriate control file: “cloud.inp”

Relevant control parameters: “Phase function of cloud layers”, “Expansion coefficients input file”, “Type of input integral parameter”, “Input integral parameter”, “Cloud particle profile input file”, “Cloud layer types”

Phase function moments and single scattering albedo

In order to use phase function moments from a pre-calculated data base, the “Phase function of cloud layers” control parameter has to be set to “mie”. In this case the program will read phase function moments from the data base appropriate to the selected type of the cloud which is to be specified in “Cloud layer types” input line. The valid inputs for “Cloud layer types” parameter are “Water- $\{\text{effective radius}\}$ ”, where effective radius of water droplets can be set to: 4, 6, 8, 10, 12, 14, 16, 18, or 20 μm , i.e., for example, entry “Water-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 .

Setting “Phase function of cloud layers” to “hg” or “isotropic”, 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 data base or to an isotropic phase function, respectively.

Limitations:

- control parameter “Delta-M or Delta-Fit” can be only set to “D-M”, see Section 3.18.1.

To supply a user-defined phase function, the “Phase function of cloud layers” control parameter has to be set to “user” and the name of the file containing the extinction coefficient, scattering coefficient, and moments of the phase function (see, for example, “Legandre.6.dat”) is to be specified as the first entry in the “Expansion coefficients input file” control line. The input file must contain a line with “>” as the first symbol, which separates the header from the data block. The first line below this separation line must contain two values which will be interpreted as the extinction and the scattering coefficients, respectively, and used to calculate the single scattering albedo for the cloud layer. This line is followed by a two-column data block containing the expansion coefficients of the phase function in the second column. The first column is ignored. The file has to be located in “./data/clouds/” directory.

Attention:

- Both file names in the “Expansion coefficients input file” control line, the first for the water and the second for the ice clouds, must always be present independent of the desired cloud type.

The values for the single scattering albedo obtained along with the phase function moments either from the pre-calculated data base or from the user-supplied file are only used if “Type of input integral parameter” is set to “TAU” (see below).

Scattering and extinction coefficients

The method used to calculate scattering and extinction coefficients depends on the setting of “Type of input integral parameter”.

For a water cloud “Type of input integral parameter” can be set to “TAU”, “TAU_TO_PATH”, “TAU_TO_DENS”, “WATER_PATH”, “LWC_PROFILE”, or “DENS_PROFILE”.

These modes are described below in details.

- “TAU” - a cloud layer is characterized by its optical thickness, τ , which is defined by the first input value (“TAU” field) in the “Input integral parameter” control line, the second and third values (“LWP” and “IWP” fields) in this control line must be present but will not be used in calculations. The control parameter “Cloud particle profile input file” should be set either to “./data/clouds/cld_prof.hom” or to “./data/clouds/cld_prof.vin”.

The program uses only the second column in this file containing the shape of the extinction coefficient profile, $Sh(z)$. This shape is defined by an arbitrary constant profile for a vertically homogeneous cloud layer or by a desired shape profile in arbitrary units for a vertically inhomogeneous cloud layer. At least 3 altitude levels must be defined in the shape file.

The vertical profile of the extinction coefficient, $\sigma_e(z)$, is calculated from the above discussed input parameters according to the following formula: $\sigma_e(z) = \tau * Sh(z) / \int_{h_b}^{h_t} Sh(z) dz$. The vertical profile of the scattering coefficient, $\sigma_s(z)$, is then given by $\sigma_s(z) = \sigma_e(z) * \omega$, where the single scattering albedo, ω , is obtained from a pre-calculated data base or from the user-supplied file, as described above.

Limitations:

- scattering and absorption coefficients are independent of the effective radius of water droplets
- single scattering albedo is constant within a cloud layer (in the absence of gaseous absorption) although scattering and absorption coefficients may be altitude dependent;
- “TAU_TO_PATH” - a cloud layer is characterized by its optical thickness, τ , which is defined by the first input value (“TAU” field) in the “Input integral parameter” control line, the second and third values (“LWP” and “IWP” fields) in this control line must be present but will not be used in calculations. The actual value for the liquid water path (LWP) needed in this mode will be calculated to match the total optical thickness of the cloud layer with the value specified by user. The control parameter “Cloud particle profile input file” should be set either to “./data/clouds/cld_prof.hom” or to “./data/clouds/cld_prof.vin”.

The program reads the second and the third columns in this file. The second column is interpreted as a shape of the liquid water content profile, $Sh^{lwc}(z)$. This shape is defined by an arbitrary constant profile for a vertically homogeneous cloud layer or by a desired shape profile in arbitrary units for a vertically inhomogeneous cloud layer. The third column in the input file is supposed to contain a vertical profile of the effective radius

of water droplets, $r_{wd}(z)$. This profile is defined by a desired constant effective radius of water droplets in μm for a vertically homogeneous cloud layer or by a desired vertical profile of the effective radius of water droplets in μm for a vertically inhomogeneous cloud layer. At least 3 altitude levels must be defined in the input file.

After the value for the liquid water path, LWP , appropriate to the specified optical thickness, τ , is found, the vertical profile of the liquid water content is calculated according to the following formula: $LWC(z) = LWP * Sh^{lwc}(z) / \int_{h_b}^{h_t} Sh^{lwc}(z) dz$. The scattering and extinction coefficients are then calculated by the program using $r_{wd}(z)$, $LWC(z)$, and the refraction index of the liquid water employing approximate formulas as described in [20].

- “TAU_TO_DENS” - same as described above for the “TAU_TO_PATH” mode but the second column in files “./data/clouds/cld_prof.hom” and “./data/clouds/cld_prof.vin” is interpreted as a shape of the particle density profile, $Sh^N(z)$.
- “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 third values (“TAU” and “IWP” fields) in this control line must be present but will not be used in calculations. The actual value of the optical thickness of the cloud layer, τ , will be calculated based on the specified value for the liquid water path. The control parameter “Cloud particle profile input file” should be set either to “./data/clouds/cld_prof.hom” or to “./data/clouds/cld_prof.vin”.

The program reads the second and the third columns in this file. The second column is interpreted as a shape of the liquid water content profile, $Sh^{lwc}(z)$. This shape is defined by an arbitrary constant profile for a vertically homogeneous cloud layer or by a desired shape profile in arbitrary units for a vertically inhomogeneous cloud layer. The third column in the input file is supposed to contain a vertical profile of the effective radius of water droplets, $r_{wd}(z)$. This profile is defined by a desired constant effective radius of water droplets in μm for a vertically homogeneous cloud layer or by a desired vertical profile of the effective radius of water droplets in μm for a vertically inhomogeneous cloud layer. At least 3 altitude levels must be defined in the input file.

The vertical profile of the liquid water content is calculated from the above discussed input parameters according to the following formula: $LWC(z) = LWP * Sh^{lwc}(z) / \int_{h_b}^{h_t} Sh^{lwc}(z) dz$. The scattering and extinction coefficients are then calculated by the program using $r_{wd}(z)$, $LWC(z)$, and the refraction index of the liquid water employing approximate formulas as described in [20].

- “LWC_PROFILE” - a cloud layer is characterized by the liquid water concentration profile. The integral parameters, which are defined in the “Input integral parameter” control line, must be present but will not be used in calculations.

The actual values of the optical thickness of the cloud layer, τ , and of the liquid water path, LWP , will be calculated based on the specified value for the liquid water content. The control parameter “Cloud particle profile input file” should be set to “./data/clouds/cld_prof.hom” or “./data/clouds/cld_prof.vin”.

The program reads the second and the third columns in this file. The second column is interpreted as a liquid water content profile, $Sh^{lwc}(z)$, in $[g/m^3]$. The third column in the

input file is supposed to contain a vertical profile of the effective radius of water droplets, $r_{wd}(z)$. This profile is defined by a desired constant effective radius of water droplets in μm for a vertically homogeneous cloud layer or by a desired vertical profile of the effective radius of water droplets in μm for a vertically inhomogeneous cloud layer. At least 3 altitude levels must be defined in the input file.

The scattering and extinction coefficients are calculated by the program using $r_{wd}(z)$, $LWC(z)$, and the refraction index of the liquid water employing approximate formulas as described in [20].

- “DENS_PROFILE” - a cloud layer is characterized by the vertical profile of water droplet density, $N(z)$. The integral parameters, which are defined in the “Input integral parameter” control line, must be present but will not be used in calculations.

The actual values of the optical thickness of the cloud layer, τ , and of the liquid water path, LWP , will be calculated based on the specified value for $N(z)$. The control parameter “Cloud particle profile input file” should be set to “../data/clouds/cld_prof.hom” or “../data/clouds/cld_prof.vin”.

The program reads the second and the third columns in this file. The second column is interpreted as a water droplet density profile, $Sh^N(z)$, in $[cm^{-3}]$. The third column in the input file is supposed to contain a vertical profile of the effective radius of water droplets, $r_{wd}(z)$. This profile is defined by a desired constant effective radius of water droplets in μm for a vertically homogeneous cloud layer or by a desired vertical profile of the effective radius of water droplets in μm for a vertically inhomogeneous cloud layer. At least 3 altitude levels must be defined in the input file.

The scattering and extinction coefficients are calculated by the program using $r_{wd}(z)$, $N(z)$, and the refraction index of the liquid water employing approximate formulas as described in [20].

3.18.3 Ice clouds

Appropriate control file: “cloud.inp”

Relevant control parameters: “Phase function of cloud layers”, “Expansion coefficients input file”, “Type of input integral parameter”, “Input integral parameter”, “Cloud particle profile input file”

Phase function moments and single scattering albedo

No pre-calculated data base is available for ice clouds.

To supply a user-defined phase function, the control parameter “Phase function of cloud layers” has to be set to “user” and a name of the file containing the extinction coefficient, scattering coefficient, and moments of the phase function (see, for example, “fractal.dat”) is to be specified as the second entry in the “Expansion coefficients input file” control line. The input file must contain a line with “>” as the first symbol, which separates the header from the data block. The first line below this separation line must contain two values which will be interpreted as the extinction and the scattering coefficients, respectively, and used to calculate

the single scattering albedo for the cloud layer. This line is followed by a two-column data block containing the expansion coefficients of the phase function in the second column. The first column is ignored. The file has to be located in “./data/clouds/” directory.

The values for the single scattering albedo obtained along with the phase function moments from the user-supplied file are only used if “Type of input integral parameter” is set to “TAU” (see below).

Attention:

- Both file names in the “Expansion coefficients input file” control line, the first for the water and the second for the ice clouds, must always be present independent of the desired cloud type.

Scattering and extinction coefficients

The method used to calculate scattering and extinction coefficients depends on the setting of “Type of input integral parameter”. For an ice cloud “Type of input integral parameter” can be set to “TAU”, “TAU_TO_PATH”, or “WATER_PATH”. These modes are described below in details.

- “TAU” - a cloud layer is characterized by its optical thickness, τ , which is defined by the first input value (“TAU” field) in the “Input integral parameter” control line, the second and third values (“LWP” and “IWP” fields) must be present but will not be used in calculations. The control parameter “Cloud particle profile input file” should be set to “./data/clouds/cld_prof.hom” or “./data/clouds/cld_prof.vin”.

The program uses only the fourth column in the input file containing the shape of the extinction coefficient profile, $Sh(z)$. This shape is defined by an arbitrary constant profile for a vertically homogeneous cloud layer or by a desired shape profile in arbitrary units for a vertically inhomogeneous cloud layer. At least 3 altitude levels must be defined in the shape file.

The vertical profile of the extinction coefficient, $\sigma_e(z)$, is calculated from the above discussed input parameters according to the following formula: $\sigma_e(z) = \tau * Sh(z) / \int_{h_b}^{h_t} Sh(z) dz$. The vertical profile of the scattering coefficient, $\sigma_s(z)$, is then given by $\sigma_s(z) = \sigma_e(z) * \omega$, where the single scattering albedo, ω , is obtained from the user-supplied file, as described above.

Limitations:

- scattering and absorption coefficients are independent of the effective radius of ice crystals;
- single scattering albedo is constant within a cloud layer (in the absence of gaseous absorption) although scattering and absorption coefficients may be altitude dependent;

- “TAU_TO_PATH” - a cloud layer is characterized by its optical thickness, τ , which is defined by the first input value (“TAU” field) in the “Input integral parameter” control line, the second and third values (“LWP” and “IWP” fields) must be present but will not be used in calculations. The actual value for the ice water path (IWP) needed in this mode will be calculated to match the total optical thickness of the cloud layer with the value specified by user. The control parameter “Cloud particle profile input file” should be set to “./data/clouds/cld_prof.hom” or “./data/clouds/cld_prof.vin”.

The program reads the fourth and the fifth columns in the input file. The fourth column is interpreted as a shape of the ice water content profile, $Sh^{iwc}(z)$. This shape is defined by an arbitrary constant profile for a vertically homogeneous cloud layer or by a desired shape profile in arbitrary units for a vertically inhomogeneous cloud layer. The fifth column in the input file is supposed to contain a vertical profile of the effective radius of ice crystals, $r_{ic}(z)$. This profile is defined by a desired constant effective radius of ice crystals in μm for a vertically homogeneous cloud layer or by a desired vertical profile of the effective radius of ice crystals in μm for a vertically inhomogeneous cloud layer. At least 3 altitude levels must be defined in the input file.

After a value for the ice water path, IWP , appropriate to the specified optical thickness, τ , is found, the vertical profile of the liquid water content is calculated according to the following formula: $IWC(z) = IWP * Sh^{iwc}(z) / \int_{h_b}^{h_t} Sh^{iwc}(z) dz$. The scattering and extinction coefficients are then calculated by the program using $r_{ic}(z)$, $IWC(z)$, and the refraction index of the ice employing approximate formulas as described in [20].

- “WATER_PATH” - a cloud layer is characterized by the ice water path, IWP , which is defined by the third input value (“IWP” field) in the “Input integral parameter” control line, the first and second values (“TAU” and “LWP” fields) must be present but will not be used in calculations. The actual value of the optical thickness of the cloud layer, τ , will be calculated based on the specified value for the ice water path. The control parameter “Cloud particle profile input file” should be set to “./data/clouds/cld_prof.hom” or “./data/clouds/cld_prof.vin”.

The program reads the fourth and the fifth columns in this file. The fourth column is interpreted as a shape of the ice water content profile, $Sh^{iwc}(z)$. This shape is defined by an arbitrary constant profile for a vertically homogeneous cloud layer or by a desired shape profile in arbitrary units for a vertically inhomogeneous cloud layer. The fifth column in the input file is supposed to contain a vertical profile of the effective radius of ice crystals, $r_{ic}(z)$. This profile is defined by a desired constant effective radius of ice crystals in μm for a vertically homogeneous cloud layer or by a desired vertical profile of the effective radius of ice crystals in μm for a vertically inhomogeneous cloud layer. At least 3 altitude levels must be defined in the input file.

The vertical profile of the ice water content is calculated from the above discussed input parameters according to the following formula: $IWC(z) = IWP * Sh^{iwc}(z) / \int_{h_b}^{h_t} Sh^{iwc}(z) dz$. The scattering and extinction coefficients are then calculated by the program using $r_{ic}(z)$, $IWC(z)$, and the refraction index of the ice employing approximate formulas as described in [20].

3.18.4 Mixed clouds (ice/water mixture)

Appropriate control file: “cloud.inp”

Relevant control parameters: “Phase function of cloud layers”, “Expansion coefficients input file”, “Input integral parameter”, “Cloud particle profile input file”

Phase function moments

No pre-calculated data base is available for mixed clouds.

To supply a user-defined phase function, the control parameter “Phase function of cloud layers” has to be set to “user” and names of the files containing extinction coefficients, scattering coefficients and moments of the phase functions for the liquid water and ice (see, for example, “Legandre_6.dat” and “fractal.dat”) are to be specified as the first and the second entries in the “Expansion coefficients input file” control line, respectively. The files must be in the same format as discussed in Sections 3.18.2 and 3.18.3 and have to be located in “./data/clouds/” directory.

Scattering and extinction coefficients

Setting of the “Type of input integral parameter” control parameter has no effect for mixed clouds.

A cloud layer is characterized by the liquid and ice water paths, LWP and IWP , which are defined by the second (“LWP” field) and the third (“IWP” field) input values in the “Input integral parameter” control line, respectively. The first value (“TAU” field) in this control line must be present but will not be used in calculations. The actual value of the optical thickness of the cloud layer, τ , will be calculated based on the specified values for the liquid and ice water paths. The control parameter “Cloud particle profile input file” should be set to “./data/clouds/cld_prof.hom” or “./data/clouds/cld_prof.vin”.

The program reads columns from the second to the fifth in the input file. The second and the fourth columns are interpreted as shapes of the liquid and ice water content profiles, $Sh^{lwc}(z)$ and $Sh^{iwc}(z)$, respectively. These shapes are defined by arbitrary constant profiles for a vertically homogeneous cloud layer or by desired shape profiles in arbitrary units for a vertically inhomogeneous cloud layer. The third and the fifth columns in the input file are supposed to contain vertical profiles of the effective radii of water droplets and of ice crystals, $r_{wd}(z)$ and $r_{ic}(z)$, respectively. These profiles are defined by desired constant effective radii of water droplets and of ice crystals, respectively, in μm for a vertically homogeneous cloud layer or by desired vertical profiles of the effective radii of water droplets and of ice crystals, respectively, in μm for a vertically inhomogeneous cloud layer. At least 3 altitude levels must be defined in the input file.

The vertical profiles of the liquid and ice water content are calculated from the above discussed input parameters according to the following formulas: $LWC(z) = LWP * Sh^{lwc}(z) / \int_{h_b}^{h_t} Sh^{lwc}(z) dz$ and $IWC(z) = IWP * Sh^{iwc}(z) / \int_{h_b}^{h_t} Sh^{iwc}(z) dz$. The scattering and extinction coefficients are then calculated by the program using $r_{wd}(z)$, $r_{ic}(z)$, $LWC(z)$, $IWC(z)$, and the refraction indexes of the liquid water and ice employing approximate formulas as described in [20].

3.19 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. It 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 3.3).

3.20 Control output

Appropriate control files: “control.inp”, “SCIATRAN_SCENARIO.OUT”, “CLIMATOLOGY.OUT”, “AEROSOL.OUT”, “errors.log”

Relevant control parameters: “Verbosity level”

The level of details in the screen output is controlled by the “Verbosity level” input parameter. This parameter consist of two characters controlling independently the screen output from the radiative transfer model (the first character) and from the retrieval block (the second character). The following settings are accepted:

- “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.

Additionally to the screen output, most important settings used for the radiative transfer modeling and for the retrieval (if appropriate) are stored in the “./DATA_OUT/SCIATRAN_SCENARIO.OUT” file, whereas the “./DATA_OUT/AEROSOL.OUT” file contains a short summary of the employed aerosol settings.

If “Do specification by geolocation” control parameter is set to “t” (see Section 3.14), an extra file “./DATA_OUT/CLIMATOLOGY.OUT” will be written out containing input settings which will be automatically changed according to the selected date and geolocation.

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 “`Verbosity level`” 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`

3.21 Output files

All data files described in this section are located in “`./DATA_OUT/`” subdirectory of main program directory. At each program run “`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 3.3) and the sphericity mode (see Section 3.2) in brackets, i.e., “`DOM, spherical mode`” means that the Discrete Ordinate solver was used for the spherical atmosphere:

```
# SCIATRAN 2.2 (DOM, spherical mode)
```

- Subsequent lines in the header contain the name of products generated in the last program run and corresponding filenames, for example:

```
# Intensity: intensity.dat
# Weighting functions: wf_o3.dat wf_temp.dat wf_press.dat wf_albedo.dat
```

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:

```
# Num.; 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;
- 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 2.2 (DOM, spherical mode)
# Intensity: intensity.dat
# Weighting functions: wf_o3.dat wf_temp.dat wf_press.dat wf_albedo.dat
# Num.; SZA, LOS angle, azimuth angle (@ TOA); output altitude
  1  70.00   0.00  30.41  100.00
  2  75.00   0.00  30.41  100.00
  3  80.05   0.00  30.41  100.00
```

Dependent on the RTM mode selected in the “RTM Mode” control line (see Section 3.4) 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 a normal user.

3.21.1 Intensity/radiance (“RTM Mode” is set to “int”)

The calculated intensity/radiance is stored in “intensity.dat” file containing the following information:

- The second line of the header contains the product name, i.e., “Radiance”, followed by the output units in brackets: “sun normalized” if “Absolute radiance” was set to “f” or “photons/s/nm/cm2/ster” if “Absolute radiance” was set to “t” (see Section 3.7).
- 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.

3.21.2 Weighting functions (“RTM Mode” is set to “wf”)

Intensity/radiance is stored in “intensity.dat” file as described in Section 3.21.1. Weighting function for the selected parameters (see Section 3.4.2) 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 in brackets: “sun normalized” if “Absolute radiance” was set to “f” or “photons/s/nm/cm2/ster” if “Absolute radiance” was set to “t” (see Section 3.7), 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 fourth lines of the header contain information on the selected spectral range and the number of output spectral points, respectively.
- The fifth 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 3.21.1). 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.

3.21.3 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 3.4.3) 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 3.21.1). 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.

3.21.4 Block air mass factors (“RTM Mode” is set to “block_amf”)

Block air mass factors for the selected atmospheric trace gas (see Section 3.4.3) are stored in “block_amf.dat” file having the same structure as weighting function files (see Section 3.4.2) with an appropriate product name in the second header line.

3.21.5 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 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 as “`intensity.dat`” (see Section 3.21.1) with an appropriate product name in the second header line.

3.21.6 Spherical albedo (“RTM Mode” is set to “`spher_alb`”)

The reflected and transmitted spherical albedos (“`spher_alb_up.dat`”, “`spher_alb_dn.dat`”) are written out. These files have the following structure:

- 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.

3.21.7 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 3.12.4), 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.inp`” 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 3.3), 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 in the subsequent columns.

3.21.8 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 3.21.1) with an appropriate product name in the second header line.

Chapter 4

Retrieval using SCIATRAN

4.1 General information

Setting “RTM Mode” parameter to “ret” (see Sec. 3.4) 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 spectra 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 [31] is employed as the default retrieval approach at the main retrieval stage. According to this approach the following equation has to be solved:

$$\hat{\mathbf{y}} = \mathbf{K}\hat{\mathbf{x}} + \epsilon, \quad (4.1)$$

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

$$\mathbf{x} = \mathbf{x}_0 + (\mathbf{K}^T \mathbf{S}_y^{-1} \mathbf{K} + \mathbf{S}_a^{-1})^{-1} \mathbf{K}^T \mathbf{S}_y^{-1} (\mathbf{y} - \mathbf{y}_0) , \quad (4.2)$$

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

$$\mathbf{A} = (\mathbf{K}^T \mathbf{S}_y^{-1} \mathbf{K} + \mathbf{S}_a^{-1})^{-1} \mathbf{K}^T \mathbf{S}_y^{-1} \mathbf{K} \quad (4.3)$$

and

$$\mathbf{S} = (\mathbf{K}^T \mathbf{S}_y^{-1} \mathbf{K} + \mathbf{S}_a^{-1})^{-1} , \quad (4.4)$$

respectively (see [31] 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 spectra 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 or 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 [33, 34, 35].
- “`triplet`” is a special mode developed to retrieve vertical distributions of ozone using the triplet method [44]. 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 $\lambda_1=525$ nm, $\lambda_2=600$, and $\lambda_3=675$ 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 “`Wavelength 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 O₂ absorption band between 758 and 772 nm.
- “**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 O₂ 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 ~ 40 km and ~ 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 [42].
- 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 radiances 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 “**Wavelength segment info**” control field (see Sec. 3.9) are read from the data file. The original wavelength grid defined in the “**Wavelength 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 “**Wavelength 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 from 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. 3.5) 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 [31]:

$$\mathbf{x}_{i+1} = \mathbf{x}_0 + (\mathbf{K}_i^T \mathbf{S}_y^{-1} \mathbf{K}_i + \mathbf{S}_a^{-1})^{-1} \mathbf{K}_i^T \mathbf{S}_y^{-1} (\mathbf{y} - \mathbf{y}_i + \mathbf{K}_i(\mathbf{x}_i - \mathbf{x}_0)) , \quad (4.5)$$

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 priori state.

If for a particular atmospheric species no reliable a priori 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:

$$\mathbf{x}_{i+1} = \mathbf{x}_i + (\mathbf{K}_i^T \mathbf{S}_y^{-1} \mathbf{K}_i + \mathbf{S}_a^{-1})^{-1} \mathbf{K}_i^T \mathbf{S}_y^{-1} (\mathbf{y} - \mathbf{y}_i) , \quad (4.6)$$

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 altitude 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., $\text{RMS_NEW/RMS_OLD} - 1$, 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:

$$\mathbf{S}_a^{i,j} = \sigma^2 \exp \left[-\frac{|z_i - z_j|}{r_c} \right], \quad (4.7)$$

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

$$\mathbf{x}_{i+1} = \mathbf{x}_0 + (\mathbf{K}_i^T \mathbf{S}_y^{-1} \mathbf{K}_i + \mathbf{S}_r)^{-1} \mathbf{K}_i^T \mathbf{S}_y^{-1} (\mathbf{y} - \mathbf{y}_i + \mathbf{K}_i(\mathbf{x}_i - \mathbf{x}_0)), \quad (4.8)$$

where

$$\mathbf{S}_r = \mathbf{S}_a^{-1} + \mathbf{S}_t^T \mathbf{S}_t \quad (4.9)$$

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 constraints 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 “**Wavelength 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.,

$$\tilde{I}_0(\lambda) = I_0(\lambda) + I_c. \quad (4.10)$$

Since the spectral fit is performed for logarithms of signals:

$$\ln \tilde{I}_0(\lambda) = \ln(I_0(\lambda) + I_c) \approx \ln I_0(\lambda) + \frac{I_c}{I_0(\lambda)}, \quad (4.11)$$

where only first two terms of the Taylor 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 “**Wavelength 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 spanned 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,

$$\mathbf{x}_{i+1} - \mathbf{x}_0 = \sum_{k=1}^{N_i} \beta_{i,k} \psi_{i,k} , \quad (4.12)$$

with the expansion coefficients

$$\beta_{i,k} = \frac{\lambda_{i,k}}{n_{i,k} (1 + \lambda_{i,k})} \psi_{i,k}^T \mathbf{K}_i^T \mathbf{S}_y^{-1} \left[\mathbf{y} - \mathbf{y}_i + \mathbf{K}_i (\mathbf{x}_i - \mathbf{x}_0) \right] , \quad (4.13)$$

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:

$$n_{i,k} = \langle \mathbf{K}^T \mathbf{S}_y^{-1} \mathbf{K} \psi_{i,k}, \psi_{i,k} \rangle. \quad (4.14)$$

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 [16, 33, 13]. 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 “ASYM” (see Sec. 3.3.2) 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. 3.18);
 - “`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 $2 \times$ “`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. 3.20) 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 “`Wavelength 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. 3.21). 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/cm³) 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 “Wavelength 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 “Wavelength 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. 3.21). 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. 3.20) 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. 3.20) 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 (see 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. 3.20) is set to “**E**” or “**D**”.

Appendix A

Tools to compile the GALAHAD Quadratic Programming Library for SCIATRAN ≥ 2.2

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 >= 2.2
# First argument is the name of the output 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 ifort (PC) and xlf (IBM) compilers and can be easily extended to any other computer platform. The file can also be downloaded at www.iup.physik.uni-bremen.de/sciatran/free_downloads.

```
#####
#
# Makefile to compile the GALAHAD quadratic programming library
# for the SCIATRAN software package
#
#####
compiler = ifort
#compiler = xlf

ifeq ($(compiler),ifort)
    FC = ifort
    OBJDIR = ./OBJ_IFORT
```

```

    FFLAGS = -O3 -module $(OBJDIR) -u -w95
    F77_FLAGS = $(FFLAGS)
endif
ifeq ($(compiler),xlf)
    FC = xlf95
    OBJDIR = ./OBJ_IBM
    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)/gltr.o $(OBJDIR)/qpb.o

OBJECTS_HSL = $(OBJDIR)/ma27.o

all: $(OBJECTS_GALAHAD) $(OBJECTS_HSL)
ar rc $(OBJDIR)/libgalahad.a $(OBJECTS_GALAHAD) $(OBJECTS_HSL)
rm $(OBJECTS)

$(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
#
#####

```

Appendix B

Keyword reference list

B.1 “control.inp”

“Absolute or relative WF”	Section 3.4.2, page 21
“Absolute radiance”	Section 3.7, page 28
“Aerosol delta-M approximation”	Section 3.17, page 44
“Aerosol parameterization type”	Section 3.17, page 44
“Aerosol phase function index”	Section 3.17, page 44
“Aerosol scaling parameter”	Section 3.17, page 44
“Albedo”	Section 3.13, page 42
“Altitude grid information”	Section 3.5, page 25
“Altitude grids for photochemically active species”	Section 3.12.4, page 40
“BRDF flag”	Section 3.13, page 42
“BRDF spectral range”	Section 3.13, page 42
“Convolution for line absorber only”	Section 3.11, page 36
“Clouds present?”	Section 3.18, page 46
“Date”	Section 3.15, page 43
“Do aerosols”	Section 3.17, page 44
“Do convolution”	Section 3.11, page 36
“Do esft anti correlation” (default value: false)	Section 3.10.4, page 35
“Do P and T from standard profile file”	Section 3.12.2, page 38
“Do profiles akima interpolation”	Section 3.12.1, page 37

“Do profile latitude interpolation”	Section 3.14, page 42
“Do specification by geolocation”	Section 3.14, page 42
“Do spectral albedo from data base”	Section 3.13, page 42
“Filename user provided solar spectrum”	Section 3.7, page 28
“Height above sea level”	Section 3.5, page 25
“Internal wavelength step”	Section 3.11, page 36
“Isotopic line parameter filename”	Section 3.10.3, page 35
“Latitude & longitude”	Section 3.15, page 43
“Line absorber treatment”	Section 3.10.2, page 34
“Line absorber windows”	Section 3.10.2, page 34
“Line wing cut-off wavenumber”	Section 3.10.3, page 35
“Lower and upper boundary for WF calculation”	Section 3.4.9, page 24
“Lower and upper boundary of flux results”	Section 3.4.4, page 23
“Number of photochemically active species”	Section 3.12.4, page 40
“Other parameters - weighting functions”	Section 3.4.2, page 21
“Ozone climatology”	Section 3.12.3, page 39
“Ozone total column”	Section 3.12.3, page 39
“Parallel wavelength loop”	Section 3.19, page 56
“Path to aerosol data base”	Section 3.17, page 44
“Path to altitude grid file”	Section 3.5, page 25
“Path to climatology data base”	Section 3.14, page 42
“Path to ESFT data base”	Section 3.10.4, page 35
“Path to ozone climatology”	Section 3.12.3, page 39
“Photochemical calculations”	Section 3.12.4, page 40
“Pressure and temperature file name”	Section 3.12.2, page 38
“Profiles for photochemically active species”	Section 3.12.4, page 40
“Rayleigh depolarisation filename”	Section 3.16, page 44
“Rayleigh depolarisation value”	Section 3.16, page 44
“Rayleigh depolarisation wavelength dependent ?”	Section 3.16, page 44
“Rayleigh scattering depletion”	Section 3.16, page 44
“Rayleigh scattering index” (recommended value: 7).....	Section 3.16, page 44

“Replace tropospheric concentrations”	Section 3.12.4, page 40
“RTM-CORE”	Section 3.3, page 19
“RTM Mode”	Section 3.4, page 20
“RTM_TYPE”	Section 3.1, page 16
“Scale climatological profile”	Section 3.12.3, page 39
“Slit function HWHM”	Section 3.11, page 36
“Slit function type”	Section 3.11, page 36
“Slit function wing cut-off”	Section 3.11, page 36
“Solar zenith angle for constant profile”	Section 3.12.4, page 40
“Spectral albedo filename”	Section 3.13, page 42
“Spectral windows for line absorbers”	Section 3.10.2, page 34
“Spectroscopic line parameter filename”	Section 3.10.3, page 35
“Standard profile scenario file name”	Section 3.12.1, page 37
“Standard profile scenario for line absorbers”	Section 3.12.1, page 37
“Stop after generating CLIMATOLOGY.OUT”	Section 3.14, page 42
“Surface type”	Section 3.13, page 42
“The number of iterations”	Section 3.2.3, page 17
“Trace gas replacement profiles”	Section 3.12.2, page 38
“Trace gas selection - AMF calculation”	Section 3.4.3, page 22
“Trace gas selection - forward model”	Section 3.10, page 32
“Trace gas selection - photochemistry”	Section 3.12.4, page 40
“Trace gas selection - weighting functions”	Section 3.4.2, page 21
“Tropopause height”	Section 3.12.4, page 40
“Truncation index for delta-M approximation”	Section 3.17, page 44
“Use constant profile”	Section 3.12.4, page 40
“Verbosity level”	Section 3.20, page 56
“Wavelength segment info”	Section 3.9, page 31
“Weighting parameter”	Section 3.5, page 25
“WF integration mode”	Section 3.4.2, page 21
“WF normalization”	Section 3.4.2, page 21
“X-sections settings input file” (default: “xsections.inp”) ..	Section 3.10.1, page 33
“X-section path”	Section 3.10.1, page 33

B.2 “control_geom.inp”

“Angle selection mode”	Section 3.8.1, page 29
“Azimuth angles”	Section 3.8.1, page 29
“Do refractive geometry”	Section 3.2.4, page 18
“Do satellite”	Section 3.8.1, page 29
“Earth radius”	Section 3.2.4, page 18
“Field of view integration”	Section 3.8.1, page 29
“Field of view size”	Section 3.8.1, page 29
“Flag for user-defined output altitude”	Section 3.8.2, page 31
“Solar zenith angles”	Section 3.8.1, page 29
“The number of azimuth angles”	Section 3.8.1, page 29
“The number of solar zenith angles”	Section 3.8.1, page 29
“The number of viewing angles”	Section 3.8.1, page 29
“Type of LOS definition”	Section 3.8.1, page 29
“User-defined output altitude”	Section 3.8.2, page 31
“Viewing angles”	Section 3.8.1, page 29

B.3 “control_ac.inp”

“Accuracy criterion”	Section 3.6.4, page 27
“Adaptive grid”	Section 3.6.3, page 27
“Azimuth series flag”	Section 3.6.4, page 27
“Do only 0th harmonic for near nadir”	Section 3.6.4, page 27
“Fine grid height”	Section 3.6.2, page 26
“Fine grid start”	Section 3.6.2, page 26
“Fine grid tangent”	Section 3.6.2, page 26
“Homogeneity criteria”	Section 3.6.3, page 27
“Near nadir definition [deg]”	Section 3.6.4, page 27
“Number of Legendre moments”	Section 3.6.4, page 27
“Number of streams”	Section 3.6.4, page 27
“Scattering mode”	Section 3.6.1, page 25

“Single scattering correction”	Section 3.6.4, page 27
“SS/MS wavelength boundary”	Section 3.6.1, page 25
“The layering of line-of-sight”	Section 3.6.2, page 26
“The number of fine grid layers”	Section 3.6.2, page 26

B.4 “control_ret.inp”

“Apriori information”	Section 4.8.1, page 67
“Calculate model spectrum”	Section 4.13, page 71
“Cloud top height constraints”	Section 4.17.2, page 74
“Cloud bottom height constraints”	Section 4.17.2, page 74
“Convergence altitude region”	Section 4.7.2, page 66
“Convergence criteria”	Section 4.7.2, page 66
“Convergence for gas”	Section 4.7.2, page 66
“Correction spectra file names and shift mode”	Section 4.9, page 68
“Correlation radius”	Section 4.8.1, page 67
“CTH convergence criterion”	Section 4.17.4, page 75
“Dark current column”	Section 4.12, page 70
“Dark current correction”	Section 4.12, page 70
“Data step”	Section 4.3, page 63
“Eigenvectors decomposition”	Section 4.14, page 71
“Eigenvectors decomposition with constraints”	Section 4.14, page 71
“Experimental data file”	Section 4.3, page 63
“Geometrical cloud parameters”	Section 4.17.1, page 73
“Geometrical thickness constraints”	Section 4.17.2, page 74
“Iterations number limit”	Section 4.7, page 65
“Lower reflection”	Section 4.17.3, page 74
“Maximum retrieval height”	Section 4.11, page 70
“Model spectrum directory”	Section 4.13, page 71
“Noise generator”	Section 4.16, page 73
“Number of correction spectra”	Section 4.9, page 68

“Number of geometrical parameters”	Section 4.17.1, page 73
“Offset correction”	Section 4.9, page 68
“Outlier criterion”	Section 4.15, page 72
“Perform shift and squeeze”	Section 4.9, page 68
“Perform squeeze”	Section 4.9, page 68
“Polynomial extraction”	Section 4.10, page 69
“Polynomial order”	Section 4.10, page 69
“Profile retrieval”	Section 4.6, page 65
“Reference measurement number”	Section 4.5, page 64
“Reference spectrum”	Section 4.5, page 64
“Reject outliers”	Section 4.15, page 72
“Retrieval mode”	Section 4.2, page 62
“S/N ratio”	Section 4.8.3, page 68
“S/N ratio file”	Section 4.8.3, page 68
“S/N ratio correction factor”	Section 4.8.3, page 68
“Set maximum retrieval height”	Section 4.11, page 70
“Signal to Noise ratio mode”	Section 4.8.3, page 68
“Smoothing parameter”	Section 4.10, page 69
“Solar spectrum file”	Section 4.5, page 64
“Start and end tangent heights”	Section 4.4, page 64
“Tangent height selection”	Section 4.4, page 64
“Threshold for eigenvalues”	Section 4.14, page 71
“Tikhonov parameter”	Section 4.8.2, page 67
“Use apriori information”	Section 4.7.1, page 65

B.5 Other control files

“cloud.inp”	Section 3.18, page 46
“esft.inp”	Section 3.10.4, page 35
“low_aer.inp”	Section 3.17, page 44
“scia_aer.inp”	Section 3.17, page 44

<code>"man_aer.inp"</code>	Section 3.17, page 44
<code>"xsections.inp"</code>	Section 3.10.1, page 33

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