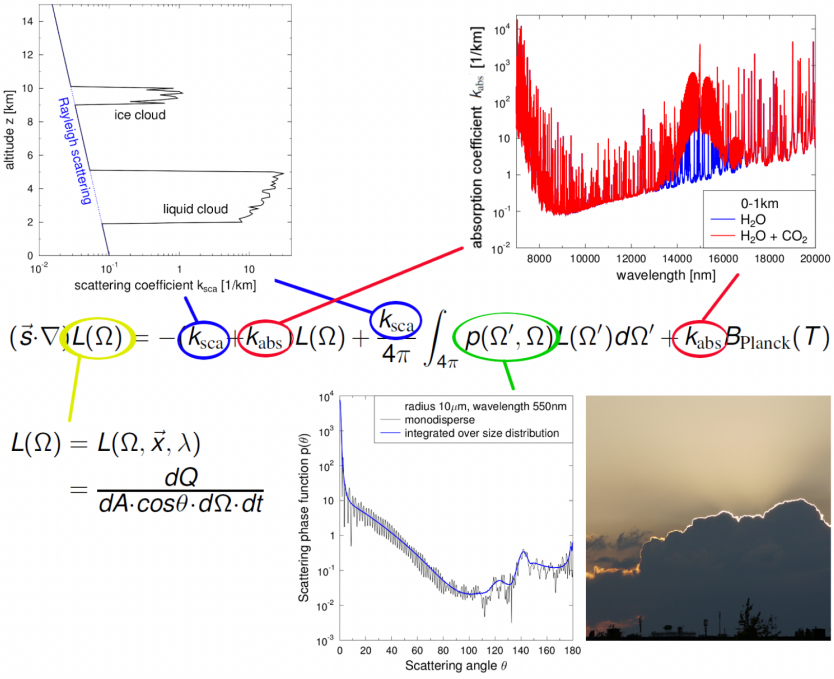
Edition for libRadtran version 2.0.6

libRadtran user's guide

Bernhard Mayer, Arve Kylling, Claudia Emde, Robert Buras,
Josef Gasteiger, Fabian Jakub, Ulrich Hamann, and Bettina Richter



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Chapter 1

Preface

libRadtran is a library of radiative transfer routines and programs. The central program of the *libRadtran* package is the radiative transfer tool *uvspec*. *uvspec* was originally designed to calculate spectral irradiance and actinic flux in the ultraviolet and visible parts of the spectrum (Kylling, 1992) where the name stems from. Over the years, *uvspec* has undergone numerous extensions and improvements. *uvspec* now includes the full solar and thermal spectrum, currently from 120 nm to 100 μm. It has been designed as a user-friendly and versatile tool which provides a variety of options to setup and modify an atmosphere with molecules, aerosol particles, water and ice clouds, and a surface as lower boundary. One of the unique features of *uvspec* is that it includes not only one but a selection of about ten different radiative transfer equation solvers, fully transparent to the user, including the widely-used DISORT code by Stamnes et al. (1988) and its C-code version (Buras et al., 2011), a fast two-stream code (Kylling et al., 1995), and the fully three-dimensional Monte Carlo code for the physically correct tracing of photons in cloudy atmospheres, MYSTIC (Mayer, 2009; Emde and Mayer, 2007; Emde et al., 2010; Buras and Mayer, 2011; Emde et al., 2011). MYSTIC optionally allows to consider polarization and fully spherical geometry. Please note that the public release includes only a 1D version of MYSTIC.

libRadtran also provides related utilities, like e.g. a Mie program (*mie*), some utilities for the calculation of the position of the sun (*zenith*, *noon*, *sza2time*), a few tools for interpolation, convolution, and integration (*spline*, *conv*, *integrate*), and several other small tools for setting up *uvspec* input and postprocessing *uvspec* output.

Further general information about *libRadtran* including examples of use may be found in the reference publication (Mayer and Kylling, 2005).

It is expected that the reader is familiar with radiative transfer terminology. In addition, a variety of techniques and parameterizations from various sources are used. For more information about the usefulness and applicability of these methods in a specific context, the user is referred to the referenced literature.

Please note that this document is by no means complete. It is under rapid development and major changes will take place.

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- The `disort` solver was developed by Knut Stamnes, Warren Wiscombe, S.C. Tsay, and K. Jayaweera
- The translation from the FORTRAN version of the DISORT solver to C-code was performed by Timothy E. Dowling
- Warren Wiscombe provided the Mie code `MIEV0`, and the routines to calculate the refractive indices of water and ice, `REFWAT` and `ICEWAT`.
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- Albano Gonzales (aglezf (at) ull.es) included the Yang et al. (2000), Key et al. (2002) ice crystal parameterization.
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Chapter 2

Radiative transfer theory

2.1 Overview

Radiative transfer in planetary atmospheres is a complex problem. The best tool for the solution may vary depending on the problem. The *libRadtran* package contains numerous tools that handle various aspects of atmospheric radiative transfer. The main tools will be presented later in chapter 3. To give the user a background for the problem to be solved, the theory behind will briefly be presented below. The radiative transfer equation is presented first, and solution methods and approximations are outlined afterwards.

The number of equations in this chapter may be intimidating even for the brave-hearted. If you just want to get things done and wonder if the *libRadtran* package includes tools that may be used for your problem, jump directly to chapter 3. Another good starting point is to try the examples available through the Graphical User Interface to the `uvspec` tool.

2.2 The radiative transfer equation

Quite generally, the distribution of photons in a dilute gas may be described by the Boltzmann equation[1]

$$\frac{\partial f}{\partial t} + \nabla_{\mathbf{r}}(\mathbf{v}\ f) + \nabla_{\mathbf{p}}(\mathbf{F}\ f) = Q(\mathbf{r}, \hat{n}, \nu, t). \tag{2.1}$$

Here, the photon distribution function $f(\mathbf{r}, \hat{n}, \nu, t)$ varies with location ($\mathbf{r}$), direction of propagation ($\hat{n}$), frequency (ν) and time (t). It is defined such that

$$f(\mathbf{r}, \hat{n}, \nu, t)\ c\ \hat{n} \cdot d\mathbf{S}\ d\Omega\ d\nu\ dt \tag{2.2}$$

represents the number of photons with frequency between ν and $\nu + d\nu$ crossing a surface element $d\mathbf{S}$ in direction $\hat{n}$ into solid angle $d\Omega$ in time dt (Stamnes 1986). The units of

[1] For a derivation of the Boltzmann equation see a textbook on statistical mechanics, for example Reif (1965). Also note that the Boltzmann equation is not a fundamental equation. For a derivation of the radiative transfer equation from the Maxwell equations see Mishchenko (2002).

$f(\mathbf{r}, \hat{n}, \nu, t)$ are $cm^{-3}\ sr^{-1}\ Hz^{-1}$ and c is the speed of light. Furthermore, $\nabla_{\mathbf{r}}$ and $\nabla_{\mathbf{p}}$ are the divergence operators in configuration and momentum space, respectively. The photons may be subject to an external force $\mathbf{F}(\mathbf{r}, \hat{n}, \nu, t)$ and there may be sources and sinks of photons due to collisions and/or 'true' production and loss, which are represented by $Q(\mathbf{r}, \hat{n}, \nu, t)$.

In the absence of relativistic effects $\mathbf{F} = 0$, and the photons propagate in straight lines with velocity $\mathbf{v} = c\ \hat{n}$ between collisions. Using the relation

$$\nabla_{\mathbf{r}}(\mathbf{v}\ f) = f\ \nabla_{\mathbf{r}}\mathbf{v} + \mathbf{v} \cdot \nabla f = \mathbf{v} \cdot \nabla f, \tag{2.3}$$

where **r** and **v** are independent variables, Eq. 2.1 may be written as

$$\frac{\partial f}{\partial t} + c\ (\hat{n} \cdot \nabla)\ f = Q(\mathbf{r}, \hat{n}, \nu, t) \tag{2.4}$$

where the **r** subscript on the gradient operator ∇ has been omitted.

The differential energy associated with the photon distribution is

$$dE = c\ h\nu\ f\ \hat{n} \cdot d\mathbf{S}\ d\Omega\ d\nu\ dt. \tag{2.5}$$

The specific intensity of photons $I(\mathbf{r}, \hat{n}, \nu, t)$ is defined such that ($\hat{n} \cdot d\mathbf{S} = \cos\theta\ dS$)

$$dE = I(\mathbf{r}, \hat{n}, \nu, t)\ dS\ \cos\theta\ d\Omega\ d\nu\ dt, \tag{2.6}$$

which gives

$$I(\mathbf{r}, \hat{n}, \nu, t) = c\ h\nu\ f(\mathbf{r}, \hat{n}, \nu, t). \tag{2.7}$$

In a steady state situation Eq. 2.4 may then be written as

$$(\hat{n} \cdot \nabla)\ I(\mathbf{r}, \hat{n}, \nu) = h\nu\ Q(\mathbf{r}, \hat{n}, \nu). \tag{2.8}$$

Eq. 2.8 may be interpreted as the radiative transfer equation in a general geometry. However, as long as the source term $Q(\mathbf{r}, \hat{n}, \nu)$ is not specified it is of little use. First, however, the two most common geometries for radiative transfer in planetary atmospheres will be described.

2.2.1 The streaming term

The streaming term $\hat{n} \cdot \nabla$ defines the geometry. In planetary atmospheres the cartesian and spherical geometries are most common. In cartesian geometry the plane-parallel approximation is often used while in spherical geometry the pseudo-spherical and spherical shell approximations are popular.

Cartesian geometry - plane-parallel atmosphere

In a Cartesian coordinate system the streaming term may be written (Rottmann, 1991; Kuo et al., 1996)

$$\begin{aligned}\hat{n}\cdot\nabla &= n_x\frac{\partial}{\partial x}+n_y\frac{\partial}{\partial y}+n_z\frac{\partial}{\partial z}\\ &= \cos\phi\sqrt{1-\mu^2}\frac{\partial}{\partial x}+\sin\phi\sqrt{1-\mu^2}\frac{\partial}{\partial y}+\mu\frac{\partial}{\partial z},\end{aligned} \tag{2.9}$$

where (n_x, n_y, n_z) are the components of the unit vector, $\mu = \cos\theta$ and ϕ is the azimuth angle.

In a plane-parallel geometry (Flat Earth approximation) the atmosphere is divided into parallel layers of infinite extensions in the x- and y-directions. This implies that there are no variation in the x- and y-directions. Hence, for this approximation the streaming term becomes

$$\hat{n}\cdot\nabla = \mu\frac{\partial}{\partial z}. \tag{2.10}$$

This approximation is used by numerous radiative transfer solvers, including the much used DISORT solver (Stamnes et al., 1988).

Spherical geometry - pseudo-spherical atmosphere

In spherical geometry the streaming term becomes[2]

$$\begin{aligned}\hat{n}\cdot\nabla &= \mu\frac{\partial}{\partial r}+\frac{1-\mu^2}{r}\frac{\partial}{\partial\mu}\\ &+\frac{\sqrt{1-\mu^2}\sqrt{1-\mu_0{}^2}}{r}\left[\cos(\phi-\phi_0)\frac{\partial}{\partial\mu_0}+\frac{\mu_0}{1-\mu_0^2}\sin(\phi-\phi_0)\frac{\partial}{\partial(\phi-\phi_0)}\right].\end{aligned} \tag{2.11}$$

In a spherically symmetric (=spherical shell) atmosphere the streaming term reduces to

$$\hat{n}\cdot\nabla = \mu\frac{\partial}{\partial r}+\frac{1-\mu^2}{r}\frac{\partial}{\partial\mu}. \tag{2.12}$$

Dahlback and Stamnes (1991) has shown that for mean intensities it is sufficient to include only the first term in Eq. 2.12 for solar zenith angles up to 90°. Thus,

$$\hat{n}\cdot\nabla = \mu\frac{\partial}{\partial r}. \tag{2.13}$$

For this to hold the direct beam must be calculated in spherical geometry. This is the so-called pseudo-spherical approximation. It may work well for irradiances, mean intensities and nadir and zenith radiances. For irradiances in off-zenith and off-nadir directions it must be shown the angle derivatives are indeed negligible. This is rarely done in practice.

[2] A derivation is provided in Appendix O of Thomas and Stamnes (1999). The appendix is available from http://odin.mat.stevens-tech.edu/rttext/.

2.2.2 The source term

The source term on the right hand side of Eq. 2.8 includes all losses and gains of radiation in the direction and frequency of interest. For photons in a planetary atmosphere the source term may be written as[3]

$$\begin{aligned} h\nu\, Q(r,\hat{n},\nu) &= h\nu\, Q(r,\theta,\phi,\nu) = -\beta^{ext}(r,\nu)\; I(r,\theta,\phi,\nu) \\ &\quad + \frac{1}{4\pi}\int_0^{\infty} \beta^{sca}(r,\nu,\nu') \int_0^{2\pi} d\phi' \int_0^{\pi} d\theta' p(r,\theta,\phi;\theta',\phi') I(r,\theta',\phi',\nu') d\nu' \\ &\quad + \beta^{abs}(r,\nu)\; B[T(r)]. \end{aligned} \tag{2.14}$$

The first term represents loss of radiation due to absorption and scattering (=extinction) out of the photon beam. The second term (multiple scattering term) describes the number of photons scattered into the beam from all other directions and frequencies, finally, the third term gives the amount of thermal radiation emitted in the frequency range of interest.

The lower part of the Earth's atmosphere, may to a good approximation, be assumed to be in local thermodynamic equilibrium [4]. Thus, the emitted radiation is proportional to the Planck function, $B[T(r)]$, integrated over the frequency or wavelength region of interest. Furthermore, by Kirchhoff's law the emissivity coefficient β^{emi} is equal to the absorption coefficient β^{abs}.

The absorption, scattering and extinction coefficients are defined as (Stamnes, 1986)

$$\beta^{abs}(r,\nu) = \sum_i \beta_i^{abs}(r,\nu), \qquad \beta_i^{abs}(r,\nu) = n_i(r)\sigma_i^{abs}(\nu) \tag{2.15}$$

$$\beta^{sca}(r,\nu) = \sum_i \beta_i^{sca}(r,\nu), \qquad \beta_i^{sca}(r,\nu) = n_i(r)\sigma_i^{sca}(\nu) \tag{2.16}$$

$$\beta^{ext}(r,\nu) = \beta^{abs}(r,\nu) + \beta^{sca}(r,\nu)$$

where $n_i(r)$ is the density of the atmospheric molecule species i and $\sigma_i^{abs}(\nu)$ and $\sigma_i^{sca}(\nu)$ are the corresponding absorption and scattering cross sections. The phase function is defined as

$$p(r,\theta,\phi;\theta',\phi',\nu) = \frac{\sum_i \beta_i^{sca}(r,\nu) p_i(\theta,\phi;\theta',\phi',\nu)}{\sum_i \beta_i^{sca}(r,\nu)}$$

where the phase function for each species

$$p_i(\theta,\phi;\theta',\phi',\nu) = p_i(\cos\Theta,\nu) = \frac{\sigma_i^{sca}(\nu,\cos\Theta)}{\int_{4\pi} d\Omega\; \sigma_i^{sca}(\nu,\cos\Theta)}$$

[3] For a derivation of the individual terms see e.g. Chandrasekhar (1960).

[4] The hypothesis of local thermodynamic equilibrium (LTE) makes the assumption that all thermodynamic properties of the medium are the same as their thermodynamic equilibrium (T.E.) values at the local T and density. Only the radiation field is allowed to depart from its T.E. value of $B[T(r)]$ and is obtained from a solution of the transfer equation. Such an approach is manifestly *internally inconsistent*. ... 'However, if the medium is subject only to *small* gradients over the mean free path a photon can travel before it is destroyed and thermalized by a collisional process, then the LTE approach is valid.' (adapted from Mihalas (1978, p. 26))

and the scattering angle Θ is related to the local polar and azimuth angles through

$$\cos\Theta = \cos\theta \ \cos\theta' + \sin\theta \ \sin\theta' \ \cos(\phi - \phi').$$

The temperature profile, the densities and absorption and scattering cross sections are all needed to solve the radiative transfer equation. Temperatures and densities may readily be obtained from measurements or atmospheric models. Cross sections are taken from measurements, from theoretical models or a combination of both.

2.2.3 The radiative transfer equation in 1D

In plane-parallel geometry the monochromatic[5] radiative transfer equation 2.8 is written by combining Eq. 2.10 and Eq. 2.14

$$\begin{aligned} -\mu\frac{dI(z,\mu,\phi)}{\beta^{ext}dz} &= I(z,\mu,\phi) \\ &\quad -\frac{\omega(z)}{4\pi}\int_0^{2\pi} d\phi' \int_{-1}^{1} d\mu' p(z,\mu,\phi;\mu',\phi') I(z,\mu',\phi') \\ &\quad -(1-\omega(z))B[T(z)] \end{aligned} \tag{2.17}$$

where the single scattering albedo

$$\omega(z) = \omega(z,\nu) = \frac{\beta_i^{sca}(z,\nu)}{\beta_i^{ext}(z,\nu)} = \frac{\beta_i^{sca}(z,\nu)}{\beta_i^{abs}(z,\nu) + \beta_i^{sca}(z,\nu)}.$$

Formally the pseudo-spherical radiative transfer equation is similar to Eq. 2.17, but with z replaced by r.

2.2.4 Polarization - scalar versus vector

The intensity or radiance I, solved for in the above equations have a magnitude, a direction and a wavelength. In addition to this light also possesses a property called polarization. When assuming randomly oriented particles the radiative transfer equation formally does not change when including polarization. However, the scalar radiance I is replaced with the vector quantity $\mathbf{I}$

$$\mathbf{I} = (I, Q, U, V), \tag{2.18}$$

where I, Q, U and V are the so-called Stokes parameters (see e.g. Bohren and Huffman (1998)). Furthermore, the phase function $p(r,\theta,\phi;\theta',\phi')$ is replaced by the 4×4 phase matrix $\mathbf{P}(r,\theta,\phi;\theta',\phi')$, and if thermal radiation is under consideration the Stokes emission vector must also be accounted for.

[5] Frequency redistribution is required if Raman scattering is included in the calculation. For many applications Raman scattering is negligible and the photons are assumed not to change frequency. They are monochromatic. Thus, all frequency dependence have been suppressed in Eq. 2.17.

The degree of polarization p is defined as

$$p = \frac{\sqrt{Q^2 + U^2 + V^2}}{I}. \tag{2.19}$$

For completely polarized radiation, $Q^2 + U^2 + V^2 = I^2$, thus $p = 1$, and for unpolarized radiation, $Q = U = V = 0$, thus $p = 0$.

In addition to the degree of polarization, p, the degree of linear polarization is defined as

$$p_{lin} = \frac{\sqrt{Q^2 + U^2}}{I}, \tag{2.20}$$

and the the degree of circular polarization is defined as

$$p_{circ} = \frac{V}{I}. \tag{2.21}$$

Polarization is often ignored in radiative transfer calculations both due to the complexity involved in the solution of the RTE including polarization and the higher demand on computer resources by these solution methods. Also, for many applications polarization may be ignored. If you are concerned about your specific application, `uvspec` makes it easy to change solvers and thus readily allows comparisons to be made between scalar and vector calculations.

2.3 General solution considerations

A multitude of methods exist to solve the radiative transfer equation 2.8. Most methods have some commonalities and they are briefly described below.

2.3.1 Direct beam/diffuse radiation splitting

The integro-differential radiative transfer equation 2.8 gives the radiance field when solved with appropriate boundary conditions, that is, the radiation incident at the bottom and the top of the atmosphere. At the bottom of the atmosphere the Earth partly reflects radiation and also emits radiation as a quasi-black-body. At the top of the atmosphere ($z = z_{\text{toa}}$) a parallel beam of sunlight with magnitude I^0 in the direction μ_0 may be present

$$I(z_{toa}, \mu) = I^0 \delta(\mu - \mu_0), \tag{2.22}$$

where $\delta(\mu - \mu_0)$ is the Dirac delta-function. It is akward to use a delta function for a boundary condition. However, a homogeneous differential equation with inhomogeneous boundary conditions may always be turned into an inhomogeneous differential equation with homogeneous boundary conditions. Since the integro-differential equation 2.8 is already inhomogeneous, the addition of another inhomogeneous term does not necessarily complicate the problem. Hence the intensity field is written as the sum of the direct (dir) and the scattered (sca)(or diffuse) radiation

$$I(z, \mu, \phi) = I^{\text{dir}}(z, \mu_0, \phi_0) + I^{\text{sca}}(z, \mu, \phi), \tag{2.23}$$

where μ_0 and ϕ_0 are the solar zenith and azimuth angles respectively. Inserting Eq. 2.23 into Eq. 2.8 it is seen that the direct beam satisfies

$$-\mu\frac{dI^{\text{dir}}(z,\mu_0,\phi_0)}{\beta^{ext}dz} = -\mu\frac{dI^{\text{dir}}(z,\mu_0,\phi_0)}{d\tau} = I^{\text{dir}}(z,\mu_0,\phi_0) \tag{2.24}$$

where the optical depth is defined as $d\tau = \beta^{ext}dz$. The scattered intensity satisfies in 1D (the sca superscript is omitted)

$$\begin{aligned} -\mu\frac{dI(\tau,\mu,\phi)}{d\tau} &= I(\tau,\mu,\phi) \\ &\quad -\frac{\omega(r)}{4\pi}\int_0^{2\pi}d\phi'\int_{-1}^{1}d\mu' p(\tau,\mu,\phi;\mu',\phi')I(\tau,\mu',\phi) \\ &\quad -(1-\omega(\tau))B[T(\tau)] \\ &\quad -\frac{\omega(\tau)I^0}{4\pi}p(\tau,\mu,\phi;\mu_0,\phi_0)e^{-\tau/\mu_0}. \end{aligned} \tag{2.25}$$

Solution of Eq. 2.24 for the direct beam yields the Beer-Lambert-Bouguer law

$$I^{dir}(\tau,\mu_0) = I^0\ e^{-\tau/\mu_0}. \tag{2.26}$$

The popular **disort** solver (Stamnes et al., 1988, 2000) solves Eqs. 2.24-2.25.

2.3.2 Pseudo-spherical approximation

In the pseudo-spherical approximation the extinction path τ/μ_0 in Eqs. 2.25 and 2.26 is replaced by the Chapman function, $ch(r,\mu_0)$ (Rees, 1989; Dahlback and Stamnes, 1991)

$$ch(r_0,\mu_0) = \int_{r_0}^{\infty}\frac{\beta^{ext}(r,\nu)\ dr}{\sqrt{1-\left(\frac{R+r_0}{R+r}\right)^2\left(1-\mu_0^2\right)}}. \tag{2.27}$$

Here R is the radius of the earth and r_0 the distance above the earth's surface. The Chapman function describes the extinction path in a spherical atmosphere.

Thus, in the pseudo-spherical approximation the direct beam is correctly described by

$$I^{dir}(r,\mu) = I^0\ e^{-ch(r,\mu_0)} \tag{2.28}$$

and the diffuse radiation is approximated by replacing the plane-parallel direct beam source in Eq. 2.25 with the corresponding direct beam source in spherical geometry

$$\begin{aligned} -\mu\frac{dI(\tau,\mu,\phi)}{d\tau} &= I(\tau,\mu,\phi) \\ &\quad -\frac{\omega(r)}{4\pi}\int_0^{2\pi}d\phi'\int_{-1}^{1}d\mu' p(\tau,\mu,\phi;\mu',\phi')I(\tau,\mu',\phi) \\ &\quad -(1-\omega(\tau))B[T(\tau)] \\ &\quad -\frac{\omega(\tau)I^0}{4\pi}p(\tau,\mu,\phi;\mu_0,\phi_0)e^{-ch(\tau,\mu_0)}. \end{aligned} \tag{2.29}$$

The **sdisort** solver included in the libRadtran software package (Mayer and Kylling, 2005) solves Eqs. 2.28-2.29.

2.3.3 Boundary conditions

The diffuse radiative transfer Eq. 2.25 is solved subject to boundary conditions at the top and bottom of the atmosphere. At the top boundary there is no incident diffuse intensity[6] ($\mu \geq 0$)

$$I(\tau = 0, -\mu, \phi) = 0. \tag{2.30}$$

The bottom boundary condition may quite generally be formulated in terms of a bidirectional reflectivity, $\rho(\mu, \phi; -\mu', \phi')$, and directional emissivity, $\epsilon(\mu)$,

$$\begin{aligned} I(\tau = \tau_g, \mu, \phi) &= \epsilon(\mu) B[T(\tau_g)] + \frac{1}{\pi}\mu_0 I_0 e^{-\tau_g/\mu_0}\rho(\mu, \phi; -\mu', \phi') \\ &\quad + \frac{1}{\pi}\int_0^{2\pi} d\phi' \int_0^1 \rho(\mu, \phi; -\mu', \phi') I(\tau, -\mu', \phi')\mu' d\mu', \end{aligned} \tag{2.31}$$

where $T(\tau_g)$ is the temperature of the bottom boundary, here the Earth's surface.

In the case of a Lambertian reflecting bottom boundary with albedo $\rho(\mu, \phi; -\mu', \phi') = A$, Eq. 2.31 simplifies to

$$\begin{aligned} \pi I(\tau_L, \mu) &= \pi\ \epsilon\ B[T(\tau_g)] + \mu_0\ A\ I^0 e^{-\tau_g/\mu_0)} \\ &\quad + 2\pi\ A \int_0^{2\pi} d\phi' \int_0^1 \mu I(\tau_L, -\mu, \phi) d\mu. \end{aligned} \tag{2.32}$$

The albedo, A, gives the fraction of reflected light under the assumption that the surface reflects radiation isotropically (Lambert reflector). The emissivity $\epsilon = 1 - A$, by Kirchhoff's law. In both Eqs. 2.31 and 2.32 the first term on the right hand side is the thermal radiation emitted by the surface. The second term is due to reflection of the direct beam that has penetrated through the whole atmosphere and the last term is reflection of downward diffuse radiation

2.3.4 Separation of the azimuthal Φ-dependence, Fourier decomposition

For scattering processes in the atmosphere the scattering phase function depends only on the angle Θ between the incident and scattered beams. This may be used to seperate out the Φ-dependence in Eqs. 2.25 and 2.29 as follows. The phase function is first expanded as a series of Legendre polynomials

$$p(\tau, \mu, \phi; \mu', \phi') = p(\tau, \Phi) = \sum_{l=0}^{2M-1} (2l + 1) g_l(\tau) p_l(\cos\Phi) \tag{2.33}$$

[6] The DISORT type RTE-solvers, **disort 1.3**, **disort 2.0**, **sdisort** and **twostr**, may include a diffuse radiation source at the top boundary. This may be of interest when for example modelling the aurora.

where the phase function moments g_l are given by

$$g_l(\tau) = \frac{1}{2}\int_{-1}^{+1} p_l(\cos\Phi)p(\tau,\Phi)d(\cos\Phi). \tag{2.34}$$

The g_1 term is called the "asymmetry factor", and $g_0 = 1$ due to normalization of the phase function. Applying the addition theorem for spherical harmonics to Eq. 2.33 gives

$$p(\tau,\Phi) = \sum_{l=0}^{2M-1}(2l+1)g_l(\tau)\left\{p_l(\mu)p_l(\mu') + 2\sum_{m=1}^{l}\Lambda_l^m(\mu)\Lambda_l^m(\mu')\cos m(\phi-\phi')\right\} \tag{2.35}$$

where the normalized associated Legendre polynomials are defined as

$$\Lambda_l^m(\mu) = \sqrt{\frac{(l-m)!}{(l+m)!}}P_l^m(\mu), \tag{2.36}$$

and $P_l^m(\mu)$ are the standard Legendre polynomials. The cosine dependence of the phase function, Eq. 2.35, suggests that cosine expansion of the intensity may be fruitful. Expanding the intensity as a cosine Fourier series:

$$I(\tau,\mu,\phi) = \sum_{l=0}^{2M-1} I^m(\tau,\mu)\cos m(\phi_0-\phi) \tag{2.37}$$

and inserting into Eqs. 2.25 and 2.29 gives $2M$ independent integro-differential equation (only the plane-parallel version is shown here)

$$\begin{aligned}
-\mu\frac{dI^m(\tau,\mu)}{d\tau} &= I^m(\tau,\mu) \\
&\quad -\frac{\omega(r)}{2}\int_{-1}^{1}d\mu'\sum_{l=m}^{2M-1}(2l+1)g_l(\tau)\Lambda_l^m(\mu)\Lambda_l^m(\mu')I^m(\tau,\mu') \\
&\quad -\delta_{m0}(1-\omega(\tau))B[T(\tau)] \\
&\quad -\frac{\omega(\tau)I^0}{4\pi}(2-\delta_{m0})\sum_{l=m}^{2M-1}(2l+1)g_l(\tau)\Lambda_l^m(\mu)\Lambda_l^m(\mu')e^{-\tau/\mu_0}.
\end{aligned} \tag{2.38}$$

where

$$\delta_{m0} = \begin{cases} 1 & \text{if } m = 0 \\ 0 & \text{if } m \neq 0 \end{cases}$$

2.3.5 Calculated quantities

Solution of the radiative transfer equation generally yields the diffuse radiance

$$I(\tau, \mu, \phi) \tag{2.39}$$

and the direct radiance

$$I^{\mathrm{d}ir}(\tau, \mu_0, \phi_0). \tag{2.40}$$

For the solvers that include polarization the vector quantities of the above quantities are calculated. From these quantities the upward, $E^+(\tau)$, and downward, $E^-(\tau)$, fluxes, or irradiances, are calculated

$$E^+(\tau) = \int_0^{2\pi} d\phi \int_0^1 \mu I(\tau, \mu, \phi) d\mu \tag{2.41}$$

$$E^-(\tau) = \mu_0 I_0 e^{-\tau/\mu_0} + \int_0^{2\pi} d\phi \int_0^1 \mu I(\tau, -\mu, \phi) d\mu. \tag{2.42}$$

Furthermore, the mean intensity

$$\overline{I}(\tau) = \frac{1}{2\pi}\left[I_0 e^{-\tau/\mu_0} + \int_0^{2\pi} d\phi \int_0^1 I(\tau, -\mu, \phi) d\mu + \int_0^{2\pi} d\phi \int_0^1 I(\tau, \mu, \phi) d\mu\right], \tag{2.43}$$

is related to the actinic flux (Madronich, 1987), F, used for the calculation of photolysis (or photodissociation) rates

$$F(\tau) = 4\pi \overline{I}(\tau). \tag{2.44}$$

Finally, heating rates may be calculated from either the flux differences or the mean intensity.

$$\frac{\partial T}{\partial t} = -\frac{4\pi}{c_p \rho_m}\frac{\partial E}{\partial z} = -\frac{4\pi}{c_p \rho_m}(1 - w)(\overline{I} - B)\frac{\partial \tau}{\partial z}. \tag{2.45}$$

Note that the partial derivative of τ with respect to z is needed since optical properties and $\overline{I}$ are calculated as functions of τ.

The various radiative transfer equation solvers included in the `uvspec` tools in the *libRadtran* package, have different capabilities to calculate the above radiative quantities. The user is referred to section 3.2 for an overview of the different solvers included in the `uvspec` program and their respective capabilities. For a complete description of all solvers with options section 6.1 should be consulted. Finally, there is nothing to complement a thorough understanding of the problem at hand, the theory behind the chosen solution and a little reading of the code itself.

2.3.6 Lidar equation

The lidar equation can be written as (see e.g. Weitkamp (2005))

$$\frac{\mathrm{d}N(r)}{\mathrm{d}r} = \frac{E_0}{E_{\mathrm{phot}}} A_{\mathrm{det}} \eta \frac{O(r)}{4\pi r^2} p(\cos\pi) \beta^{sca}(r) \exp\left(-2\int_0^r dr' \beta^{ext}(r')\right), \tag{2.46}$$

where $N(r)$ is the number of detected photons, E_0 is the energy per laser pulse, E_{phot} is the energy per photon, A_{det} is the detector area, η is the detector efficiency, $O(r)$ is the overlap function, r is the range, and $p(\cos\pi)$ is the scattering phase function in backward direction. Note that the nomenclature here is consistent with the libRadtran documentation and differs from that in most lidar papers and books.

The lidar equation is a solution of the RTE for the special problem of a lidar signal, and is a single scattering approximation to the real world. Nevertheless it is applicable for many cases of interest. For space-borne lidars it should not be used.

Many lidarists are also interested in the lidar ratio, which is defined as

$$S(r) = \frac{4\pi}{p(\cos\pi)\omega(r)}. \tag{2.47}$$

For the special case of Lambertian surface reflection, the signal is

$$N_{\mathrm{surf}}(r_{\mathrm{surf}}) = \frac{E_0}{E_{\mathrm{phot}}} A_{\mathrm{det}} \eta \frac{O(r_{\mathrm{surf}})}{4\pi r_{\mathrm{surf}}^2} 4a \cos\theta_{\mathrm{refl}} \exp\left(-2\int_0^{r_{\mathrm{surf}}} dr' \beta^{ext}(r')\right), \tag{2.48}$$

where r_{surf} is the range of the surface, a is the surface albedo, and θ_{refl} is the inclination with which the laser beam hits the surface.

2.3.7 Verification of solution methods

To solve the radiative transfer equation involves complex numerical procedures that are difficult both to develop and to implement. Great care must be taken during implementation to assure that the numerical procedure is stable for any values and combinations of the input parameters, i.e. optical depth, single scattering albedo, phase function and boundary conditions. The testing of new solvers are typically done by the developers against analytical solutions which are available for a few special cases. Furthermore, tests and comparisons are made against other models and measurements. The reader is referred to the individual papers describing the various solvers for more information.

The input quantities needed by the solvers are optical depth, single scattering albedo, phase function and boundary conditions. These are calculated from atmospheric profiles of molecular density, trace gas species, water and ice clouds and aerosols. In addition, the absorption and scattering properties of the various species are taken from measurements or model calculations. The calculation of the optical properties are compared against other models and measurements during code development.

Chapter 3

Radiative transfer simulations - *uvspec*

The *uvspec* program calculates the radiation field in the Earth's atmosphere. Input to the model are the constituents of the atmosphere including various molecules, aerosols and clouds. The absorption and scattering properties of these constituents may either be taken from the algorithms and databases provided with *libRadtran* and *uvspec* or be provided by the user. Boundary conditions are the solar spectrum at the top of the atmosphere and the reflecting surface at the bottom. Several extraterrestrial solar spectra are provided with *libRadtran* and various surface models are also included.

uvspec is structured into the following three essential parts: (1) An atmospheric shell which converts atmospheric properties like ozone profile, surface pressure, or cloud microphysical parameters into optical properties required as input to (2) the radiative transfer equation solver which calculates radiances, irradiances, actinic fluxes and heating rates for the given optical properties; and (3) post-processing of the solver output including multiplication with the extraterrestrial solar irradiance correction of Earth-Sun distance, convolution with a slit-function, or integration over wavelength (depending on the choice of the user). For an overview see Figure 3.1.

The core of all radiative transfer models is a method to calculate the radiation field for a given distribution of optical properties by solving the radiative transfer equation. To solve the radiative transfer equation discussed in Chapter 2 *uvspec* has the unique feature of giving the user a choice of various radiative transfer solvers (table 3.2). This implies that for the radiative transfer problem at hand an appropriate solver may be chosen, e.g. a fast two-stream code to calculate approximate irradiance or a discrete ordinate code to accurately simulate radiances, with or without polarization. The full 3D radiative transfer equation may be solved by the Monte Carlo solver MYSTIC. Please note that the public release includes only a 1D version of MYSTIC.

Below the basic usage of *uvspec* is described first followed by a general description of the *uvspec* input file and output file. The *uvspec* input file may either be generated manually using any text editor capable of saving files in ASCII (plain text) format, or it may be generated by the *uvspec* Graphical User Interface found in the `GUI` folder. The input/output

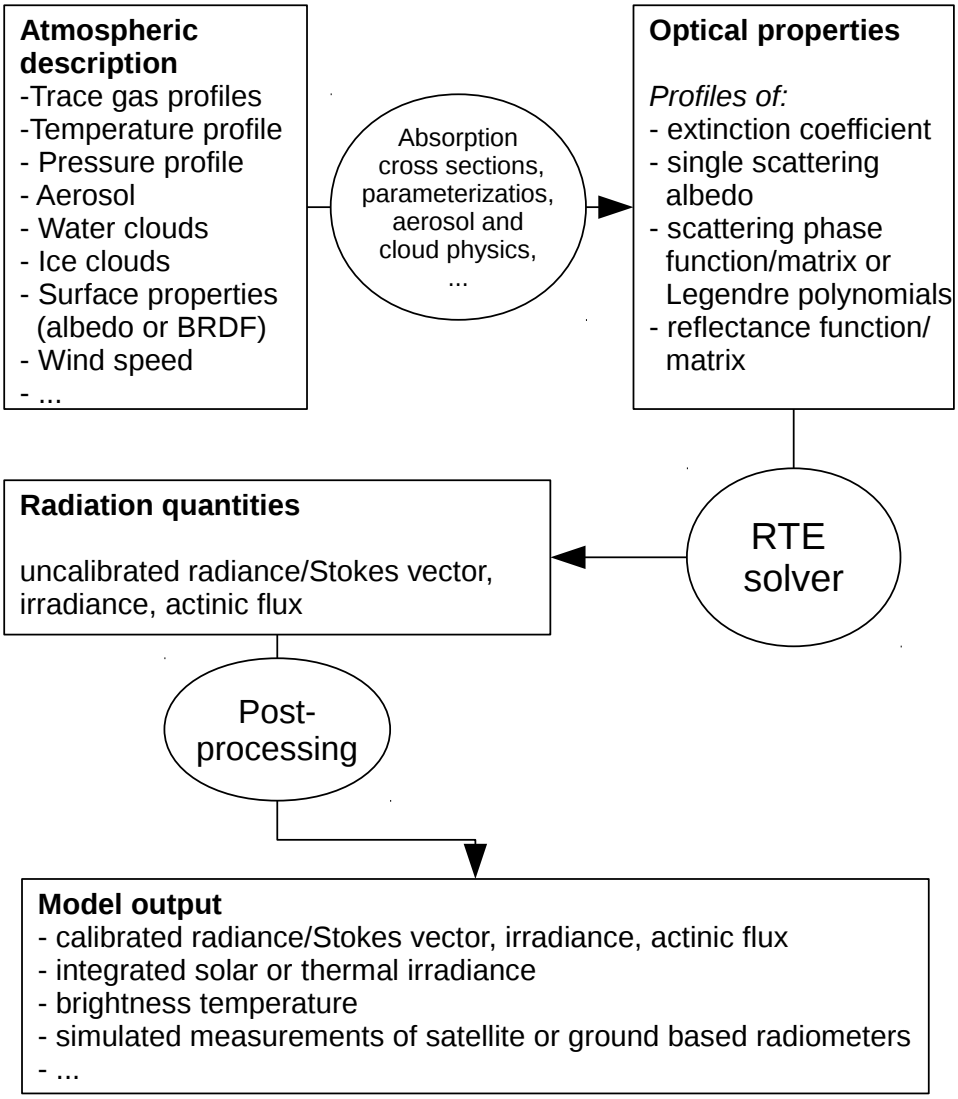

Figure 3.1: Structure of the *uvspec* model

file description is followed by a brief description of the radiative transfer equation solvers available in *uvspec*. Finally several examples of usage of *uvspec* are given.

3.1 Basic usage

3.1.1 Running *uvspec*

uvspec reads from standard input, and outputs to standard output. It is normally invoked in the following way[1]:

```
uvspec < input_file > output_file
```

The formats of the input and output files are described below. Several realistic examples of input files are given in section 3.3.

uvspec may produce a wealth of diagnostic messages and warnings, depending on your use of `verbose` or `quiet`. Diagnostics, error messages, and warnings are written to `stderr` while the *uvspec* output is written to `stdout`. To make use of this extra information, you may want to write the standard *uvspec* output to one file and the diagnostic messages to another. To do so, try `(./uvspec < uvspec.inp > uvspec.out) >& verbose.txt`. The irradiances and radiances will be written to `uvspec.out` while all diagnostic messages go into `verbose.txt`. This method can also be used to collect *uvspec* error messages.

Warning: Please note the error checking on input variables is not complete at the moment. Hence, if you provide erroneous input, the outcome is unpredictable.

3.1.2 The *uvspec* input file

uvspec is controlled in a user-friendly way. The control options are named in a (hopefully) intuitive way.

The *uvspec* input file consists of single line entries, each making up a complete input to *uvspec*. First on the line comes the option name, followed by one or more parameter values. The option name and the parameter values are separated by white space. Filenames are entered without any surrounding single or double quotes. Comments are introduced by a `#`. Blank lines are ignored. The order of the lines is not important, with one exception: if the same input option is used more than once, the second one will usually over-write the first one. Be aware that also options in another included input file will overwrite options specified before.

[1] The Graphical User Interface to *uvspec* provides another convenient way. *uvspec* may also be called as a function from another C program. See `src/worldloop.c` for an example.

3.1.3 How to setup an input file for your problem (checklist)

There are several steps to consider when setting up an input file for your specific problem. First of all we strongly recommend that you read a radiative transfer textbook to become familiar with what is required for your problem. Below is a short checklist including the steps you need to consider for each problem:

1. **Wavelength grid / band parameterization**

   By default, libRadtran employs the REPTRAN band parameterization with a spectral resolution of 15 cm^{-1}. It allows to calculate quantities integrated over narrow spectral bands. You need to specify a wavelength range using `wavelength`. The wavelengths for which the radiative transfer calculations are performed are determined by the parameterization and implicitly consider high-spectral-resolution features of molecular absorption within each band. With `wavelength_grid_file` pseudo-spectral calculations can be performed, meaning that you can calculate radiation at any wavelength you want, but it is always a weighted mean calculated from radiative transfer calculations at so-called representative wavelengths of the belonging band - if you select the wavelengths too close, you will see the steps in your spectrum. `wavelength_grid_file` is particularly useful if the default resolution is too expensive for your application. If you need a higher spectral resolution of the band data use `mol_abs_param reptran fine/medium`.

   The spectral parameterizations can be switched off with `mol_abs_param crs`. This can be necessary for example for wavelength below 205nm, or if you want to use your own high-spectral resolution atmospheric data. In this case, the radiative transfer calculations are performed on the grid provided by `wavelength_grid_file`. Finally, in order to calculate integrated shortwave or integrated longwave radiation, please choose one of the pre-defined correlated-k distributions, e.g. `mol_abs_param kato2` or `mol_abs_param fu` because these are not only much more accurate but also much faster than a pseudo-spectral calculation. Please read the respective sections in the manual to become familiar with the `mol_abs_param` options.

2. **Quantities**

   The next point one needs to consider is the desired radiation quantity. Per default, *uvspec* provides direct, diffuse downward and diffuse upward solar irradiance and actinic flux at the surface. Thermal quantities can be calculated with `source thermal` - please note that *uvspec* currently does either solar or thermal, but not both at the same time. If both components are needed (e.g. for calculations around 3μm) then *uvspec* needs to be called twice. To calculate radiances in addition to the irradiances, simply define `umu`, `phi`, and `phi0` (see next section).

3. **Geometry**

   Geometry includes the location of the sun which is defined with `sza` (solar zenith angle) and `phi0` (azimuth). The azimuth is only required for radiance calculations. Please note that not only the solar zenith angle but also the sun-earth-distance change

in the course of the year which may be considered with `day_of_year` (alternatively, `latitude`, `longitude`, and `time` may be used). The altitude of the location may be defined with `altitude` which modifies the profiles accordingly. Radiation at locations different from the surface may be calculated with `zout` which gives the sensor altitude above the ground. For satellites use `zout TOA` (top of atmosphere). For radiance calculations define the cosine of the viewing zenith angle `umu` and the sensor azimuth `phi` and don't forget to also specify the solar azimuth `phi0`. `umu`>0 means sensor looking downward (e.g. a satellite), `umu`<0 means looking upward. `phi` = `phi0` indicates that the sensor looks into the direction of the sun, `phi`-`phi0` = 180° means that the sun is in the back of the sensor.

4. **What do you need to setup the atmosphere?**

   To define an atmosphere, you need at least an `atmosphere_file` which usually contains profiles of pressure, temperature, air density, and concentrations of ozone, oxygen, water vapour, carbon dioxide, and nitrogen dioxide. The set of six standard atmospheres provided with libRadtran is usually a good start: `midlatitude_summer`, `midlatitude_winter`, `subarctic_summer`, `subarctic_winter`, `tropical`, and `US-standard`. If you don't define anything else, you have an atmosphere with Rayleigh scattering and molecular absorption, but neither clouds, nor aerosol.

   (a) **Trace gases?**

   Trace gases are already there, as stated above. But sometimes you might want to modify the amount. There is a variety of options to do that, e.g. `mol_modify O3` which modifies the ozone column, or `mixing_ratio CO2`, ...

   (b) **Aerosols?**

   If you want aerosol, switch it on with `aerosol_default` and use either the default aerosol or one of the many `aerosol_` options to setup whatever you need.

   (c) **Clouds?**

   uvspec allows water and ice clouds. Define them with `wc_file` and `ic_file` and use one of the many `wc_` or `ic_` options to define what you need. Please note that for water and ice clouds you also have a choice of different parameterizations, e.g. `ic_properties fu`, `yang`, `baum`, ...- these are used to translate from liquid/ice water content and droplet/particle radius to optical properties. You need some experience with clouds to define something reasonable. Here are two typical choices for a `wc_file 1D`

```
# z[km] LWC[g/m3] Reff[um]
    2        0        0
    1      0.1       10
```

   and an `ic_file 1D`

```
# z[km] IWC[g/m3] Reff[um]
   10        0       0
    9    0.015      20
```

The first is a water cloud with effective droplet radius of 10μm between 1 and 2 km, and an optical thickness of around 15; the second is an ice cloud with effective particle radius 20μm between 9 and 10 km and an optical thickness of about 1.

(d) **Surface properties?**

Per default, the surface albedo is zero - the surface absorbs all radiation. Define your own monochromatic albedo, a spectral `albedo_file` or a BRDF, e.g. for a water surface which is mainly determined by the wind speed `brdf_cam u10`.

5. **Choice of the radiative transfer equation (RTE) solver**

The RTE-solver is the engine, or heart, in any radiative transfer code. All RTE-solvers involve some approximations to the radiative transfer equations, or the solution has some uncertainties due to the computational demands of the solution method. The choice of RTE-solver depends on your problem. For example, if your calculations involves a low sun you should not use a plane-parallel solver, but one which somehow accounts for the spherical shape of the Earth. You may choose between many RTE-solvers in *uvspec*. The default solution method to the radiative transfer is the discrete ordinate solver `disort` which is the method of choice for most applications. There are other solvers like `rte_solver twostr` (faster but less accurate), `rte_solver sdisort` (pseudo-spherical), or `rte_solver mystic` (three-dimensional, polarization-dependent solver, spherical geometry). Even lidars can be simulated using `rte_solver sslidar`.

6. **Postprocessing**

The spectral grid of the output is defined by the extraterrestrial spectrum, which can be modified using `source solar file`. If you want spectrally integrated results, use either `output_process integrate` for `mol_abs_param lowtran` and `mol_abs_param reptran`, or `output_process sum` for `mol_abs_param kato2`. Check also other options like `filter_function_file`, `output_quantity brightness`, etc. Instead of calibrated spectral quantities you might also want `output_quantity transmittance` or `output_quantity reflectivity`.

7. **Check your input**

Last but not least, make always sure that *uvspec* actually does what you want it to do! A good way to do that is to use `verbose` which produces a lot of output. To reduce the amount, it is a good idea to do only a monochromatic calculation. Close to the end of the verbose output you will find profiles of the optical properties (optical thickness, asymmetry parameter, single scattering albedo) which give you a pretty good idea, e.g. if the clouds which you defined are already there, where the aerosol is, etc. As a general rule, never trust your input, but always check, play around, and improve. For if thou thinkest it cannot happen to me and why bother to use the verbose option, the gods shall surely punish thee for thy arrogance!

3.1.4 How to translate old input files?

Since *libRadtran* version 1.8 input option names have changed. In the directory src_py/ you will find a program translate.py to translate old style input files to new style input files.

To translate your input file use the following command:

```
python translate.py filename
```

To save the output into a new filename use:

```
python translate.py filename --new_filename=new_inputname
```

To overwrite your old input file use:

```
python translate.py filename --new_filename=filename
--force
```

3.1.5 Output from *uvspec*

The *uvspec* output depends on the radiative transfer solver. The output formats are described in the following. The meaning of the symbols is described in Table 3.1. The output may be user controlled to some degree using the option `output_user`.

disort, sdisort and spsdisort

For the disort, sdisort and spsdisort solvers *uvspec* outputs one block of data to standard output (stdout) for each wavelength.

If `umu` is not specified the format of the block is

```
lambda edir edn eup uavgdir uavgdn uavgup
```

If `umu` is specified the format of the block is

```
lambda edir edn eup uavgdir uavgdn uavgup umu(0)
u0u(umu(0)) umu(1) u0u(umu(1)) .  .  .  .
```

If both `umu` and `phi` are specified the output format of each block is

```
lambda edir edn eup uavgdir uavgdn uavgup
                              phi(0)     ...     phi(m)
umu(0)  u0u(umu(0))  uu(umu(0),phi(0))  ...  uu(umu(0),phi(m))
umu(1)  u0u(umu(1))  uu(umu(1),phi(0))  ...  uu(umu(1),phi(m))
  .          .             .                        .
  .          .             .                        .
umu(n)  u0u(umu(n))  uu(umu(n),phi(0))  ...  uu(umu(n),phi(m))
```

and so on for each wavelength.

twostr and rodents

The format of the output line for the twostr solver is

```
lambda edir edn eup uavg
```

for each wavelength.

polradtran

The polradtran solver has been deprecated. For these applications the `mystic` solver should be used. In case that you think you need a deterministic polarized solver, please get in touch with us.

mystic

Monte Carlo is the method of choice (1) for horizontally inhomogeneous problems; (2) whenever polarization is involved; (3) for applications where spherical geometry plays a role; and (4) whenever sharp features of the scattering phase function play a role, like for the calculation of the backscatter glory or the aureole. The format of the output files of the `mystic` solver is described in section 3.2.5.

sslidar

The format of the output line for the sslidar solver is

```
center-of-range number-of-photons lidar-ratio
```

for each range bin.

Description of symbols

The symbols used in section 3.1.5 are described in table 3.1.

The total downward irradiance is given by

```
eglo = edir + edn
```

The total mean intensity is given by

```
uavg = uavgdir + uavgdn + uavgup
```

If `deltam` is on it does not make sense to look at the direct and diffuse contributions to `uavg` separately since they are delta-M scaled (that is, the direct would be larger than expected and the diffuse would be smaller).

Symbol	Description
lambda	Wavelength (nm)
edir	Direct beam irradiance w.r.t. horizontal plane (same unit as extraterrestrial irradiance).
edn	Diffuse down irradiance, i.e. total minus direct beam (same unit as edir).
eup	Diffuse up irradiance (same unit as edir).
uavg	The mean intensity. Proportional to the actinic flux: To obtain the actinic flux, multiply the mean intensity by 4π (same unit as edir).
uavgdir	Direct beam contribution to the mean intensity (same unit as edir).
uavgdn	Diffuse downward radiation contribution to the mean intensity (same unit as edir).
uavgup	Diffuse upward radiation contribution to the mean intensity (same unit as edir).
u0u	The azimuthally averaged intensity at numu user specified angles umu (units of e.g. mW/(m^2 nm sr) if using the atlas3 spectrum in the data/solar_flux directory.) Note that the intensity correction included in the disort solver is not applied to u0u, thus u0u can deviate from the azimuthally-averaged intensity-corrected uu.
uu	The radiance (intensity) at umu and phi user specified angles (unit e.g. mW/(m^2 nm sr) if using the atlas3 spectrum in the data/solar_flux directory.)
uu_down, uu_up	The downwelling and upwelling radiances (intensity) at cmu and phi angles (unit e.g. mW/(m^2 nm sr) if using the atlas3 spectrum in the data/solar_flux directory.)

Table 3.1: Description of symbols used in the description of the model output.

3.2 RTE solvers included in *uvspec*

The *uvspec* tool includes numerous radiative transfer equation solvers. Below their capabilities and limitations are briefly described. A complete technical description of all solvers is far beyond the scope of the present document. The reader is referred to the individual papers describing the specific solver (see references for each solver). The solvers as they are named in the *uvspec* input files are written in **bold**. They also appear within the parenthesis in the subsection heads below. A list of all the solvers is provided in Table 3.2.

3.2.1 DIScrete ORdinate Radiative Transfer solvers (DISORT)

The discrete ordinate method was developed by Chandrasekhar (1960) and Stamnes et al. (1988). It solves the radiative transfer in 1-D geometry and allows accurate calculations of radiance, irradiance, and actinic flux. The standard DISORT solver developed by Stamnes et al. (1988, 2000) is probably the most versatile, well-tested and mostly used 1D radiative transfer solver on this planet.

The *uvspec* model includes the standard DISORT solvers which are available from `ftp://climate1.gsfc.nasa.gov/wiscombe/Multiple_Scatt/`. In addition, a number of special purpose disort-family solvers are included.

From a historic point of view it is of interest to note that the first version of *uvspec* was based on the DISORT solver.

DISORT solvers (disort, fdisort1, fdisort2)

This group of solvers solve the 1D plane-parallel radiative transfer equation 2.25. A very complete and thorough description of the nitty-gritty details of the standard DISORT solver has been provided by Stamnes et al. (2000). The theory behind is clearly elucidated by Thomas and Stamnes (1999). Three versions of the DISORT solver are included in *uvspec*.

fdisort1 The original fortran77 DISORT version 1.3.

fdisort2 The fortran77 DISORT version 2.0, with several improvements.

disort The C version of DISORT version 2.0, translated from fdisort2 by T. Dowling (Buras et al., 2011), can also be used in pseudo-spherical mode.

The major changes between version 1.3 and 2.0 includes improved treatment for peaked phase functions and a realistic handling of the bidirectional reflectance function (BRDF). The modified version `fdisort2` (and `disort`) further improves the treatment of peaked phase functions. Important improvements to the intensity correction method by Nakajima and Tanaka (1988) are described in Buras et al. (2011).

`disort` is the C version of fdisort2. The C version runs in double precision, produces less instabilities, and is slightly faster. Further, it can be used in pseudo-spherical mode.

If you are in doubt, use `disort`, which is the default RTE solver in *uvspec*. If you are worried about spherical effects please use the additional option `pseudospherical`.

Table 3.2: The radiative transfer equation solvers currently implemented in *libRadtran*.

RTE solver	Geometry	Radiation quantities	Reference	Comments
disort	1D, PP, PS	E, F, L	Buras et al. (2011)	discrete ordinate (C-version)
MYSTIC	3D, 1D, PP, SP	E, F, **I**	Mayer (2009); Emde and Mayer (2007); Emde et al. (2010); Buras and Mayer (2011); Emde et al. (2011)	Monte Carlo[(a)], polarization
fdisort1	1D, PP	E, F, L	Stamnes et al. (1988)	discrete ordinate (DISORT 1.3)
fdisort2	1D, PP	E, F, L	Stamnes et al. (2000)	discrete ordinate (DISORT 2.0)
twostr	1D, PS	E, F	Kylling et al. (1995)	two-stream; pseudo-spherical correction
rodents	1D, PP	E,F	Zdunkowski et al. (2007)	Note that the reference contains errors (see next section)
sdisort	1D, PS	E, F, L	Dahlback and Stamnes (1991)	pseudo-spherical correction, double precision, customized for airmass calculations
spsdisort	1D, PS	E, F, L	Dahlback and Stamnes (1991)	pseudo-spherical correction, single precision, not suitable for cloudy conditions
tzs	1D, PP	L(TOA)		thermal, zero scattering
sss	1D, PP	L(TOA)		solar, single scattering
sslidar	1D, PP	$*$		

[(a)] partial (1D) version included in the free package; available in joint projects

Explanation:
- PP, plane-parallel
- PS, pseudo-spherical
- SP, fully spherical
- 1D, one-dimensional
- 3D, three-dimensional
- E, irradiance
- F, actinic flux
- L, radiance
- L(TOA), radiance at top of atmosphere
- $*$ sslidar: see section 3.1.5.

I indicates the Stokes vector, L is it's first element.

Pseudo-spherical DISORT (sdisort, spsdisort)

Dahlback and Stamnes (1991) extended the DISORT version 1.3 solver to pseudo-spherical geometry by solving equation 2.25. The `sdisort` solver includes further improvements, for instance the possibility to include 2D density profiles of trace gases. This option is of importance for air mass factor (AMF) calculations relevant for analysis of DOAS measurements. The `sdisort` solver does not include the improvements of DISORT version 2.0.

Note that `sdisort` is not a fully spherical solver and may thus not be used for limb geometry.

The `spsdisort` solver is a single precision version of **sdisort**. Unless you have a 64-bit processor with compilers that do the numerics using all 64-bits we do not recommend that you use it because of numerical instabilities caused by the limited numerical resolution of 32-bits CPUs.

Two-stream solvers (twostr, rodents)

The DISORT solver are multi-stream solvers and thus not optimized for fast two-stream calculations. The `twostr` solver was developed by Kylling et al. (1995) and solves equation 2.25. Being a two-stream solution, `twostr` can not calculate radiances. Furthermore, based on the accuracy requirements of the specific application, the user is encouraged to make sample sensitivity test of `twostr` results versus for example `sdisort`.

Note that you need to use the option `pseudospherical` in order to use the solver described in Kylling et al. (1995), else you are using the plane-parallel version.

The `rodents` solver is the delta-Eddington twostream method presented in Zdunkowski et al. (2007), Sect. 6. Note that the equations (6.50) and (6.88) in the reference are wrong. Also note that the thermal radiation is not implemented as described on page 178 of the reference, but in analogy to the solar radiation. The solver was implemented by Robert Buras, hence the name "ROberts' Delta-EddingtoN Two-Stream".

3.2.2 Polarization (polradtran)

The polradtran solver has been deprecated. The `polradtran` solver developed by Evans and Stephens (1991) solves the plane-parallel RTE including polarization in 1D. It should be noted that `polradtran` is not accurate for strongly peaked phase functions that are typical for water and ice cloud scattering in the shortwave spectral region. For these applications the `mystic` solver should be used.

3.2.3 Thermal zero scattering (tzs)

The `tzs` solver developed by Luca Bugliaro is a fast solver to calculate thermal radiances at the top of the atmosphere for a non-scattering atmosphere. It may also be used to calculate "black cloud" radiances. The cloud top heights can be specified using the option

`tzs_cloud_top_height`. `tzs` has been used to apply the so called CO_2 slicing algorithm for the determination of cloud top temperatures from satellite based passive remote sensing measurements.

3.2.4 sslidar

The solver basically returns the solution of the lidar equation (2.46) and the lidar ratio, Eq. (2.47). The overlap function is set to 1. Input parameters for this solver are:

sslidar area Detector area in units of m^2 (default: $1m^2$)

sslidar E0 Energy of laser pulse in units of J (default: 0.1J)

sslidar eff Detector efficiency (default: 0.5)

sslidar position Altitude of position of lidar in units of km (default: 0km)

sslidar range width of range bin in units of km (default: 0.1km)

sslidar_nranges Number of range bins (default: 100)

Also, the cosine of the nadir angle into which the lidar is shooting/looking can be set using the option `umu` (default: 0).

The result is evaluated in the center of each range bin, i.e. the extinction from one range bin to the next is integrated correctly up to the middle of the range bin, where the backscatter coefficient is evaluated. This is then multiplied with the width of the range bin in order to get the number of photons detected in this range bin. The lidar ratio is also evaluated in the center of each range bin.

3.2.5 Three-dimensional RTE solver (mystic)

The Monte Carlo method is the most straightforward way to calculate (polarized) radiative transfer. In forward tracing mode individual photons are traced on their random paths through the atmosphere. Starting from top of the atmosphere (for solar radiation), or being thermally emitted by the atmosphere or surface, the photons are followed until they hit the surface or leave again at top of the atmosphere (TOA). For solar radiation, the start position is either a random location in the TOA plane, with the direction determined by the solar zenith and azimuth. Originally, the "Monte Carlo for the physically correct tracing of photons in cloudy atmospheres" MYSTIC (Mayer, 2009) has been developed as a forward tracing method for the calculation of irradiances and radiances in plane-parallel atmospheres. Later the model has been extended to fully spherical geometry and a backward tracing mode (Emde and Mayer, 2007). The backward photon tracing option speeds up the calculation of radiances and allows very fast calculations in the thermal spectral range.

MYSTIC is now a full vector code: It can handle polarization and polarization-dependent scattering by randomly oriented particles, i.e. clouds droplets and particles, aerosol particles, and molecules (Emde et al., 2010). To keep the computational time reasonable for

accurate calculations of e.g. polarized radiances in cloudy atmospheres several "tricks" are required to speed up the calculations. The first is the so called "local estimate method" (Marshak and Davis, 2005). Using this method a photon contributes to the final result of the calculation each time it is scattered. However, in the presence of particles with strong forward scattering in the simulated scene, such as clouds and large aerosols, the local estimate method will produce so-called "spikes", these are rare photons whose very large contribution to the result leads to slow convergence. The spike problem can be resolved by using the "Variance Reduction Optimal Options Method" (VROOM, Buras and Mayer, 2011), a collection of several variance reduction methods which change the photon paths such that the spikes disappear, but without altering the result (i.e. the variance reduction is "unbiased").

A detailed introduction to the Monte Carlo technique and in particular to MYSTIC is given in Mayer (2009). For specific questions concerning the Monte Carlo technique the reader is referred to the literature (Marchuk et al., 1980; Collins et al., 1972; Marshak and Davis, 2005; Cahalan et al., 2005).

MYSTIC is switched on by the option `rte_solver mystic`. If no other options are specified MYSTIC computes unpolarized quantities for a plane-parallel atmosphere. If `mc_polarisation` is specified, polarized quantities are computed. The option `mc_spherical 1D` enables calculations in a 1D spherical model atmosphere. All MYSTIC-specific options start with `mc_` and are described in detail in section 6.1.

MYSTIC output

uvspec will print its output (horizontally averaged irradiance and actinic flux) usually to stdout. MYSTIC provides several additional output files. We have to distinguish two classes of output: Monochromatic and spectral output where the latter can be recognized by the extension ".spc". Monochromatic output files

- mc.flx - irradiance, actinic flux at levels
- mc.rad - radiance
- mc.abs - absorption/emission
- mc.act - actinic flux, averaged over layers

are generated only for the case of a calculation where MYSTIC is called only once. That is, a monochromatic calculation without subbands introduced by `mol_abs_param`. They contain "plain" MYSTIC output, without consideration of extraterrestrial irradiance, sun-earth-distance, spectral integration, etc. As such they are mainly interesting for MYSTIC developers or for users interested in artificial cases and photon statistics since they are as close as possible to the photon statistics of MYSTIC: e.g. the "irradiance" in these files is basically the number of photons arriving at the detector divided by the number of photons traced. In addition to the average, a standard deviation of the result can be calculated online which is stored in ".std".

For most real-world applications the user will prefer the ".spc" files

- mc.flx.spc - spectral irradiance, actinic flux at levels
- mc.rad.spc - spectral radiance at levels
- ...

In contrast to the monochromatic files which are transmittances (E/E0, L/E0, ...) the data in ".spc" is "fully calibrated" output, as for all other solvers. "fully calibrated" means multiplied with the extraterrestrial irradiance, corrected for the Sun-Earth distance, integrated/summed over wavelength, etc. Please be aware that such a calculation might require a lot of memory because output is stored as a function of x, y, z, and wavelength (and possibly polarization, if you switched on `mc_polarisation`). E.g. a comparatively harmless "mol_abs_param kato2" calculation with an sample grid of 100x100 pixels at 10 altitudes would imply about 100x100x10x148 = 14,800,000 (Nx·Ny·Nz·Nlambda) grid points. Depending on the output chosen (irradiance, radiance, ...) up to six floating point numbers need to be stored which amounts to 360 MBytes. Depending on the post-processing in *uvspec*, this memory may actually be used twice which then would be 720 MBytes.

mc.flx / mcNN.flx The output file `mc.flx` contains the irradiance at the surface defined by elevation file. Note that this output is **not** for $z = 0$, but for the actual 2D surface:

```
500  500 0 0.325889 0 0 0.441766 0
500 1500 0 0.191699 0 0 0.267122 0
500 2500 0 0.210872 0 0 0.420268 0
```

The columns are:

1. x [m] (pixel center)
2. y [m] (pixel center)
3. direct transmittance
4. diffuse downward transmittance
5. diffuse upward transmittance
6. direct actinic flux transmittance
7. diffuse downward actinic flux transmittance
8. diffuse upward actinic flux transmittance

The transmittance is defined as irradiance devided by the extraterrestrial irradiance. It is not corrected for Sun-Earth-Distance.

Note that even for an empty atmosphere, the transmittance would not be 1 but cos(SZA), due to the slant incidence of the radiation.

The output files `mcNN.flx` contain the irradiances at different model levels - one for each `zout`. `NN` is the number of the output level counted from the bottom (ATTENTION: Levels are counted from 0 here!). The file format is the same as in `mc.flx`.

(If interested in surface quantities, please use the irradiance data at the surface from `mc.flx`, not from `mc00.flx`; the data from `mc00.flx` or whatever layer coincides with the surface may be wrong for technical reasons).

mc.rad / mcNN.rad The output file `mc.rad` contains the radiance at the surface defined by `elevation_file`. Note that this output is **not** for $z = 0$, but for the actual 2D surface:

```
500  500 45 270 0.0239094 0 0.0623305 0.063324
500 1500 45 270 0.0239094 0 0.0602891 0.063156
```

The columns are:

1. x [m] (pixel center)
2. y [m] (pixel center)
3. viewing zenith angle [deg]
4. viewing azimuth angle [deg]
5. aperture solid angle [sterad]
6. direct radiance component
7. diffuse radiance component
8. "escape" radiance

For almost all applications you may safely ignore the “direct” and “diffuse” radiance components and use only the escape radiance. If the latter is 0 then you probably forgot to switch on `mc_escape`. The "escape" radiance is the radiance "measured" by an ideal instrument with 0° opening angle. It is only calculated when `mc_escape` is selected and it usually converges much faster than the "cone sampled" radiance in column 7. It is recommended to always use `mc_escape` for radiance calculations. For the “direct” and “diffuse” radiance, photons falling into the aperture are counted. This might be an option for instruments with a very large aperture only because otherwise the result is noisy.

The output files `mcNN.rad` contain the radiances at different model levels - one for each `zout`. `NN` is the number of the output level counted from the bottom (ATTENTION: Levels are counted from 0 here!). The file format is the same as in `mc.rad`.

(If interested in surface quantities, please use the radiance data at the surface from `mc.rad`, not from `mc00.rad`; the data from `mc00.rad` or whatever layer coincides with the surface may be wrong for technical reasons).

mcNN.abs The file `mcNN.abs` includes the absorption per unit area in the given layer. NN is the number of the output layer on the atmospheric grid (counted from the bottom, starting from 1). This file is generated if `mc_forward_output heating` is specified.

The columns are:

1. x [m] (pixel center)
2. y [m] (pixel center)
3. heating rate (W/m^2)

If multiplied by the extraterrestrial irradiance, the heating rate in W/m^2 is obtained. In a 1D atmosphere heating rate = e_net(top) - e_net(bottom).

For computational efficiency reasons `mcNN.abs` is not provided on the sample grid but on the atmospheric grid. For the same reason, results are only calculated for 3D layers. In order to obtain 3D absorption for 1D cloudless layer, you need to specify an optically very thin 3D cloud, e.g. LWC/IWC = 10^{-20} g/m^3 (yes, this is a dirty trick but a necessary one).

mcNN.act `mcNN.act` contains the 4π actinic flux in the given layer, calculated from the absorbed energy (per unit area) divided by the absorption optical thickness of the layer. In contrast to the actinic flux in `mcNN.flx`, this is a layer quantity the accuracy of which is generally much better than the level quantities which are calculated from radiance / cos (theta). As for the absorption above, `mcNN.act` is not provided on the sample grid but on the atmospheric grid. NN is the number of the output layer (counted from the bottom, starting from 1). This file is generated if `mc_forward_output actinic` is specified.

The columns are:

1. x [m]
2. y [m]
3. actinic flux (W/m^2)

The spectral files are as follows:

mc.flx.spc :

```
 400.0 0 0 0 1.0e+00 0.0e+00 1.5067e-01 1.0e+00 0.0e+00 3.5044e-01
 401.0 0 0 0 1.0e+00 0.0e+00 1.5044e-01 1.0e+00 0.0e+00 3.5863e-01
 402.0 0 0 0 1.0e+00 0.0e+00 1.5022e-01 1.0e+00 0.0e+00 3.4755e-01
```

The columns are:

1. wavelength [nm]
2. ix (0 ... Nx-1)
3. iy (0 ... Ny-1)
4. iz (0 ... Nz-1)
5. direct irradiance
6. diffuse downward irradiance
7. diffuse upward irradiance
8. direct actinic flux
9. diffuse downward actinic flux
10. diffuse upward actinic flux

These numbers are created the same way as the standard *uvspec* output. That is, they are multiplied with the extraterrestrial irradiance, corrected for Sun-Earth-distance, integrated over wavelength, converted to reflectivity or brightness temperature, etc.

mc.rad.spc :

```
400.0 0 0 0 0.0398276
401.0 0 0 0 0.0396459
402.0 0 0 0 0.0398005
```

The columns are:

1. wavelength [nm]
2. ix (0 ... Nx-1)
3. iy (0 ... Ny-1)
4. iz (0 ... Nz-1)
5. radiance

These numbers are created the same way as the standard *uvspec* output. That is, they are multiplied with the extraterrestrial irradiance, corrected for Sun-Earth-distance, integrated over wavelength, converted to reflectivity or brightness temperature, etc.

If the **polarized** mystic is used (`mc_polarisation`) then the four components of the Stokes vector (I,Q,U,V) are output for each wavelength and grid point, in four separate lines.

3.3 Examples

In the following sections, several examples are given, how to create an input file, how to define a cloudless sky atmosphere, how to add aerosols and clouds, etc. All examples are taken from the libRadtran examples directory and are part of the *uvspec* self-check. For a complete listing and explanation of all input options, have a look at section 6.1. More examples of *uvspec* input files (extension `.INP`) are found in the `examples` directory. Several examples are also availabe through the *uvspec* Graphical User Interface (see `GUI` directory).

3.3.1 Cloudless, aerosol-free atmosphere

The simplest possible input file contains only a few lines:

```
                          # Location of atmospheric profile file.
atmosphere_file ../data/atmmod/afglus.dat

                          # Location of the extraterrestrial spectrum
source solar ../data/solar_flux/atlas_plus_modtran

wavelength 310.0 310.0    # Wavelength range [nm]

quiet
```

The first two statements define the location of some data files: the the atmospheric profile (`atmosphere_file`), and the extraterrestrial spectrum (`source solar file`). The third line defines the desired wavelength range which is a monochromatic data point in this example. All other data which are not explicitely mentioned assume a default value which is "0" in most cases. Here, the solar zenith angle is 0, the surface albedo is 0, and the atmosphere does not contain clouds nor aerosols. Pressure, temperature, ozone concentration, etc. are read from `atmosphere_file`.

An example of a more complete input file for a clear sky atmosphere is:

```
                          # Location of atmospheric profile file.
atmosphere_file ../data/atmmod/afglus.dat
                          # Location of the extraterrestrial spectrum
source solar ../data/solar_flux/atlas_plus_modtran
mol_modify O3 300. DU     # Set ozone column
day_of_year 170           # Correct for Earth-Sun distance
albedo 0.2                # Surface albedo
sza 32.0                  # Solar zenith angle
rte_solver disort         # Radiative transfer equation solver
number_of_streams  6      # Number of streams
wavelength 299.0 341.0    # Wavelength range [nm]
slit_function_file ../examples/TRI_SLIT.DAT
                          # Location of slit function
spline 300 340 1          # Interpolate from first to last in step

quiet
```

It is helpful to know some details about the **input/output wavelength resolution** in *uvspec* and how it can be influenced by the user. Basically there are three independent wavelength grids, the **input grid**, the **internal grid**, and the **output grid**. Note, that the internal grid is separated in two individual grids when REPTRAN is used, as described below. The essential thing to know is that the internal grid is chosen by *uvspec* itself in a reasonable way, if not explicitely defined in the input file with `wavelength_grid_file` or `mol_tau_file abs`. The output grid is completely independent of the internal grid and is entirely defined by `source solar file` or `source thermal file`. The wavelength grids of all other input data (e.g. albedo, optical properties of aerosols and clouds, etc) are also completely independent. These data are automatically interpolated to the resolution of the internal wavelength grid. Hence, only two constraints are set to the gridding of the input data: (1), the wavelength range has to cover all internal grid points;

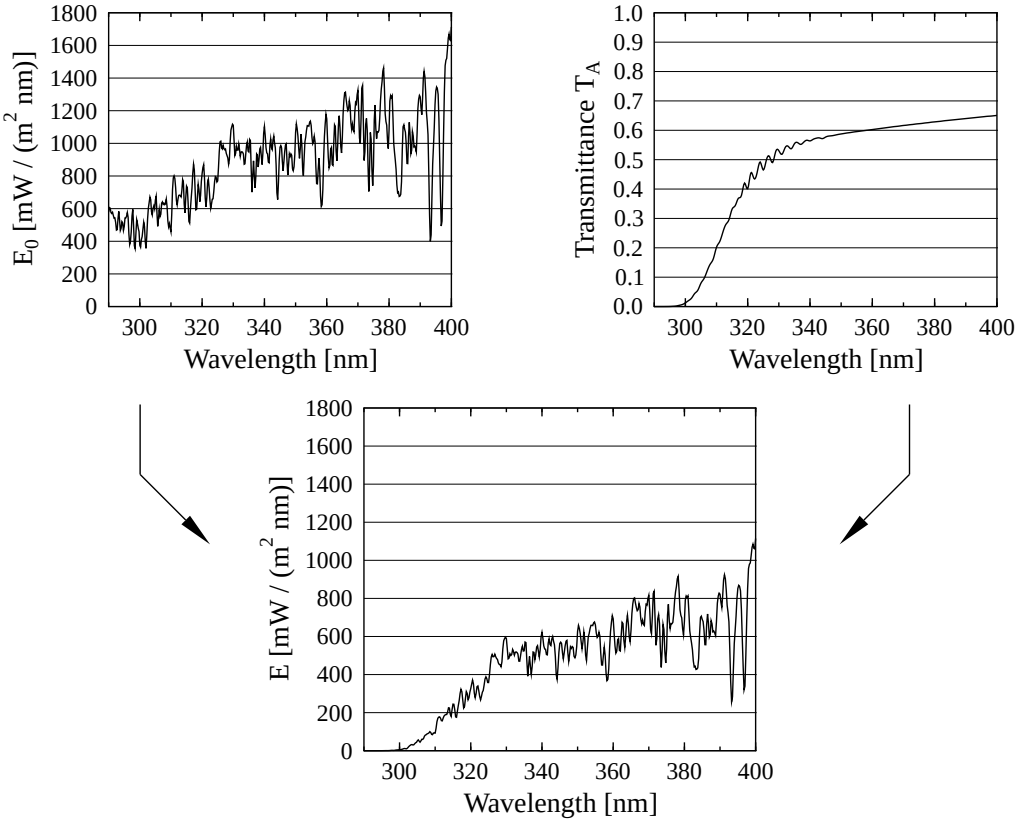

Figure 3.2: *uvspec* calculation of spectral irradiance in the ultraviolet range. (Top left) High-resolution extraterrestrial irradiance Kurucz (1992), averaged over 0.1 nm intervals. (Top right) Low-resolution atmospheric transmittance for US standard atmosphere, solar zenith angle 0°. (Bottom) Product of both: spectral irradiance.

and (2), it should be chosen in a reasonable manner to allow reasonable interpolation (which essentially means, dense enough).

For spectrally resolved calculations (`mol_abs_param crs`) in the ultraviolet/visible, *uvspec* uses an internal grid with a step width of 0.5nm below 350nm and 1nm above 350nm. This is a conservative choice which fully resolves the broad ozone absorption bands and the slowly varying Rayleigh, aerosol, and cloud extinctions. The idea is outlined in figure 3.2 which is taken from Mayer et al. (1997).

The transmittance (or reflectance) is calculated on a moderate resolution grid which reduces the number of calls to the `rte_solver` and hence the computational time. Then, the transmittance is interpolated to the wavelengths in the `source solar file` (which is usually defined with higher spectral resolution), multiplied with the extraterrestrial irradiance, and possibly post-processed. Hence, the wavelength in the output spectrum are those contained in the `source solar file` which has two important implications: (1) Only those wavelengths are output that are contained in the `source solar file`. If e.g. a monochromatic calculation is defined by setting

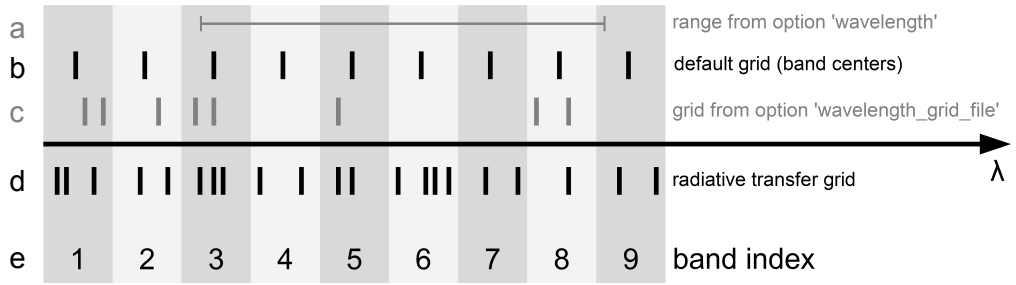

Figure 3.3: Example for internal wavelength grids when using `mol_abs_param reptran` (see text for details); the shaded areas illustrate the spectral ranges of the different parameterized adjacent non-overlapping bands.

'`wavelength 327.14`', there will only be output if the wavelength 327.14 is explicitely listed in `source solar file`; (2) this is also true at thermal wavelengths where the extraterrestrial irradiance is zero; hence, even for a calculation in the thermal range a `source thermal file` can be specified which defines the output grid in the first column and arbitrary values in the second column. Keeping these points in mind, `source solar/thermal file` is a convenient way to define an arbitrary output grid. `file` may be omitted for thermal radiation calculations (`source thermal`), representative wavelength calculations (`mol_abs_param reptran`), as well as for `output_quantity transmittance` and `output_quantity reflectivity` calculations. If omitted, the output grid equals the internal wavelength grid.

If required, a **user-defined internal grid** can be specified with `wavelength_grid_file` or `mol_tau_file abs`. Note that this is a way to speed up the calculation considerably. E.g., for some applications the internal grid in the UV-A and visible can be set to 10nm which would reduce computational times by up to a factor of 10.

Things are completely different if a k distribution method is selected (see below). In this case all flexibility is taken away from the user which is an inherent feature of the k distribution method. Internal grid as well as the extraterrestrial file are in this case defined by the choice of the parameterization itself.

If the band parameterization REPTRAN is used, two internal grids exist, as illustrated in Fig. 3.3: The first internal grid (above arrow) by default is defined by the wavelengths at the centers of the bands (line b of Fig. 3.3). The wavelength range is selected using the `wavelength` option (line a of Fig. 3.3); all bands overlapping with the specified wavelength range are modeled, for example bands 3 to 9 in Fig. 3.3. The first internal grid can be specified directly by the user with `wavelength_grid_file` option (line c of Fig. 3.3). The second internal grid consists of the representative wavelengths where the radiative transfer calculations are performed (line d of Fig. 3.3). The representative wavelengths grid is created automatically for all bands required for the first internal grid; for example, the second internal grid contains only the representative wavelengths required for

bands 1, 2, 3, 5, and 8 for the `wavelength_grid_file` illustrated in line c of Fig. 3.3. After the radiative transfer calculations are finished, transmittances calculated at the second internal grid are converted to transmittances at the first internal grid according to the weighting given by the parameterization. The transmittances at the first internal grid are used for further processing, i.e. to calculate the results on the output grid.

3.3.2 Spectral resolution

uvspec offers five different ways of spectral calculations:

1. **Spectrally resolved calculation** in the UV and visible spectral ranges;
2. **Line-by-line calculation** with user-defined molecular absorption data;
3. **The correlated-k method**;
4. **Representative wavelengths** parameterization for spectral calculations and satellite channels as described by Gasteiger et al. (2014); *uvspec* uses this approach by default;
5. **Pseudo-spectral calculation** with exponential-sum-fit, from LOWTRAN; code adopted from SBDART (Ricchiazzi et al., 1998).

The choice of the method is determined by the problem and the decision is therefore entirely up to the user. The spectrally resolved calculation and the line-by-line calculation are more or less exact methods while the correlated-k distribution, the pseudo-spectral calculation, and representative wavelength method are approximations that provide a compromise between speed and accuracy. In the following it is briefly described which method fits which purpose:

A **spectrally resolved calculation** is the most straightforward way, and is a good choice for all users interested in the ultraviolet and visible spectral ranges. This method is activated by the input option `mol_abs_param crs`. In the UV/VIS gas absorption generally occurs in broad bands with only slow spectral variation, the most important of these being the Hartley, Huggins, and Chappuis bands of ozone. Hence, a radiative transfer calculation every 1nm usually is sufficient to fully resolve any spectral variation using the method described in the last section. Absorption cross sections for various species are included, among them the most important O3 and NO2.

In the infrared, however, molecular absorption spectra are characterized by thousands of narrow absorption lines. There are two ways to treat these, either by highly resolved spectral calculations, so-called **line-by-line** calculations, or by a band parameterization. Concerning line-by-line, *uvspec* offers the possibility to define a spectrally resolved absorption cross section profile using `mol_tau_file abs`. There is no option in libRadtran to generate such a `mol_tau_file abs`, because (1) the HITRAN database which forms the basis for such calculations amounts to about 100 MByte which are updated continuously; and (2), there are sophisticated line-by-line programs available, like e.g. ARTS (Eriksson et al., 2011). Using ARTS it is straightforward to create the input for *uvspec* line-by-line calculations since it provides an option to write the absorption optical thicknesses in the required format. Line-by-line cross sections available for the six standard profiles that come

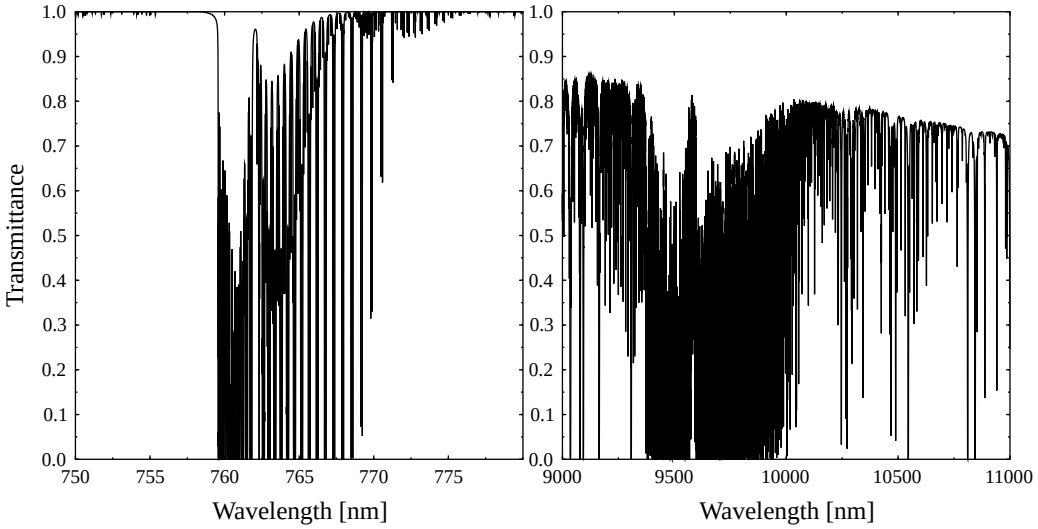

Figure 3.4: Line-by-line calculation of the atmospheric transmittance in two selected solar and thermal spectral ranges, the O2A-absorption band around 760 nm and a region within the infrared window around 10 μm.

with libRadtran are also available on request. Figure 3.4 shows an example of a line-by-line calculation of the atmospheric transmittance in two selected solar and thermal spectral ranges, the O2A-absorption band around 760 nm and a region within the infrared window around 10 μm.

All spectral lines in the left figure are due to absorption by oxygen, while the ones in the right figure are due to ozone, water vapour, and CO2. Line-by-line is obviously the exact way for radiation calculations. For most applications, however, line-by-line is far too slow. Here one needs a band parameterization. *uvspec* contains several **correlated-k parameterizations** which are invoked with `mol_abs_param`, in particular Kato et al. (1999); Fu and Liou (1992); Kratz and Varanasi (1995), as well as the possibility to specify a user-defined one. Kato et al. (1999) is a accurate parameterization for the solar spectral range. *uvspec* contains three different versions:

Kato
: The original tables provide by Seiji Kato which should correspond to the full version described in Kato et al. (1999); 575 subbands total, that is, 575 calls to the `rte_solver`

Kato2
: A new, optimized version of the tables, provided by Seiji Kato, 2003, with only 148 subbands (that is, calls to the `rte_solver`); the uncertainty is only slightly higher than `Kato`; the absorption coefficients are based on HITRAN 2000.

Kato2.96
: Similar to `Kato2` but based on HITRAN96.

Figure 3.5 shows a comparison between the three parameterization which are part of li-

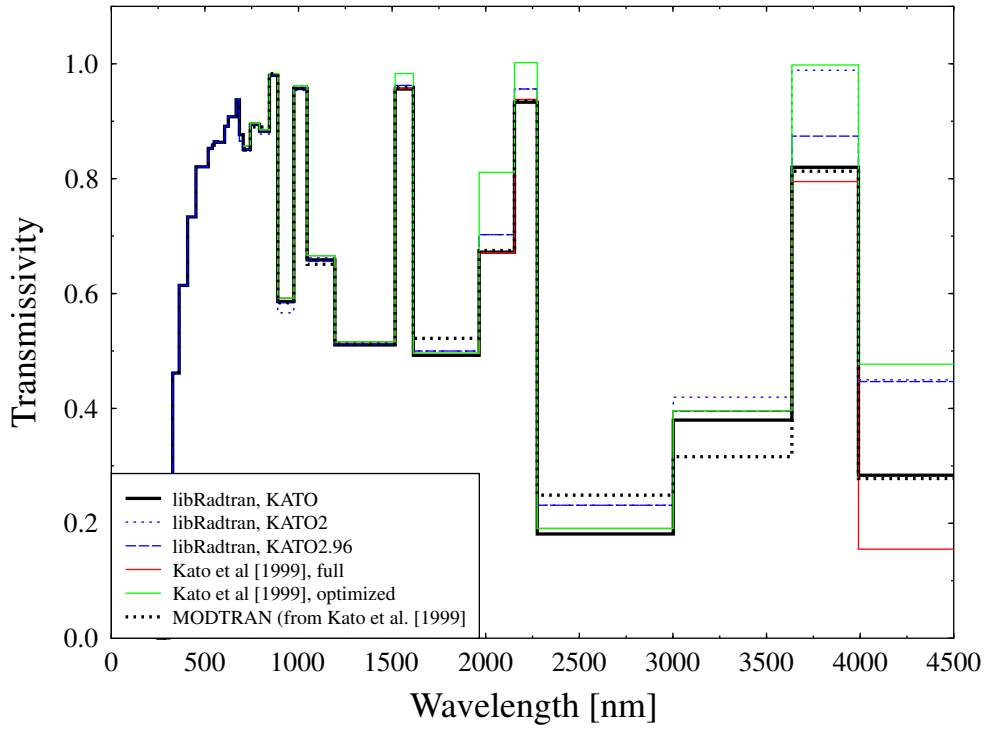

Figure 3.5: Comparison between the three parameterization which are part of *uvspec* and the data from Figure 3 by Kato et al. (1999).

bRadtran and the data from Figure 3 by Kato et al. (1999). It is immediately obvious that the uncertainty is high for all bands above 2.5 micrometer which is probably due to the treatment of band overlap. For this reasons, the results for the indiviudal bands should not be trusted while the integrated shortwave radiation (the sum of all 32 bands) is calculated with high accuracy because (1) the bands above 2.5 micrometer contribute only little to the integrated irradiance; and (2) errors are random and cancel each other to some degree.

For more information on these parameterizations please refer to the mentioned publications. Correlated-k is a powerful way to calculate spectrally integrated quantities, however, it takes away some flexibility. In particular, this means that the wavelength grid is no longer chosen by the user but by the parameterization, that is, by *uvspec*. The *uvspec* output is then no longer spectral quantities, e.g. W/(m^{2}nm), but integrated over the spectral bands, e.g. W/m^2.

A simple but complete example for a correlated-k approximation of the solar spectrum:

```
# Conditions for the calculation of Figure 3 in
# Kato et al., JQSRT 62, 109-121, 1999.
# To compare the data, the direct irradiance calculated
# by uvspec has to be divided by cos(30 deg) because
# Kato et al. plot direct normal irradiance.

                          # Location of atmospheric profile file.
atmosphere_file ../examples/AFGLMS50.DAT
                          # Location of the extraterrestrial spectrum

albedo 0.2                # Surface albedo
sza 30.0                  # Solar zenith angle
rte_solver twostr        # Radiative transfer equation solver
pseudospherical

mol_abs_param KATO        # Correlated-k by Kato et al. [1999]

output_process sum        # Calculate integrated solar irradiance

quiet
```

Here, the solar spectrum is split up into 32 bands according to Kato et al. (1999). In order to calculate integrated shortwave irradiance, simply sum the outputs, or even simpler, add `output_process sum` to the input file.

As an molecular absorption parameterization, we have implemented the **representative wavelength approach** (REPTRAN) in the solar and thermal spectral range. REPTRAN is used as the default spectral approach in *uvspec*. Parameterized bands are available for spectral calculations. Furthermore a number of satellite channels have been parameterized in addition (available with `mol_abs_param reptran_channel`). The approach is described by Buehler et al. (2010) and Gasteiger et al. (2014). The required data files are available at the libRadtran homepage. Band- and channel-integrated quantities are parameterized by weighted sums of these quantities calculated at a few representative wavelengths. Solar bands are parameterized in the spectral range from 395 nm to 5000 nm, thermal bands from 2.5 μm to 100 μm. For both solar and thermal bands different spectral resolutions are available and can be selected using `mol_abs_param reptran coarse|medium|fine` (default: `coarse`). `fine` corresponds to a band width of 1 cm^{-1}, whereas widths of 5 cm^{-1} and 15 cm^{-1} are used by `medium` and `coarse`, respectively. The solar band parameterizations are extended by 15 cm^{-1} wide bands from 240 nm to 395 nm, where only a single representative wavelength (band center) is used for each band.

Figure 3.6 shows the results of solar and thermal calculations from 395 nm to 100 μm. The water vapour absorption bands in the solar range are clearly visible, as is the absorption window around 10 μm in the thermal.

An example which calculates fluxes at the ground in the solar range is available in `examples/UVSPEC_REPTRAN_SOLAR.INP`:

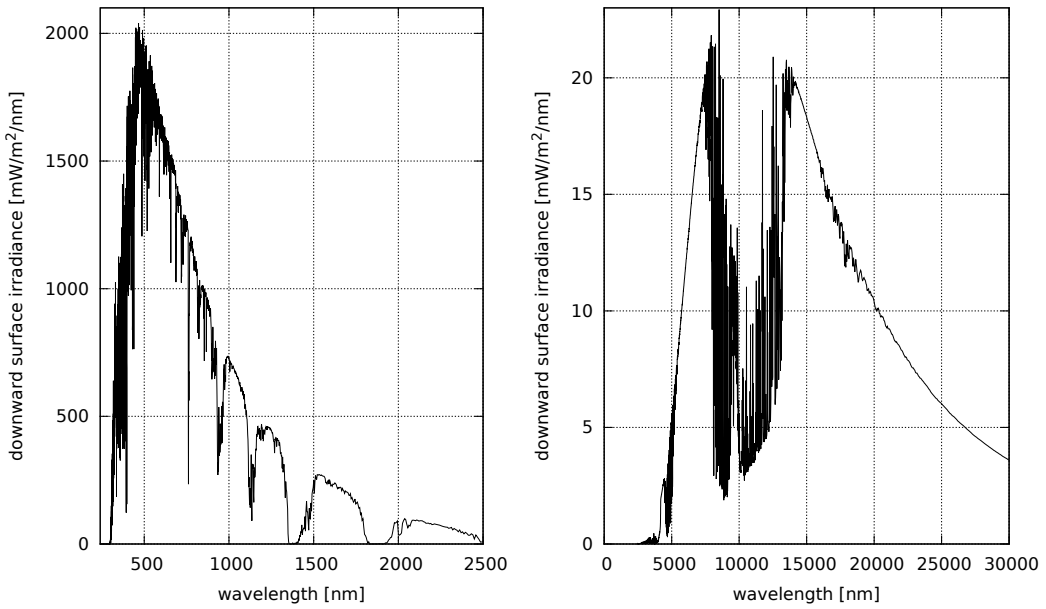

Figure 3.6: Results of solar and thermal calculations using `mol_abs_param reptran` for US standard atmosphere.

```
rte_solver twostr        # Radiative transfer equation solver

# Uncomment the following line to use finer spectral resolution
# for wavelength > 395nm

#mol_abs_param reptran fine

source solar             # solar

wavelength 300 3000   # Reptran allows for 120nm to 5000nm

quiet
```

Internally, the extraterrestrial flux from Kurucz (1992) is applied, thus no `source solar file` is required.

The default unit for solar fluxes is mW/(m^{2}nm), and for thermal fluxes is W/(m^{2}cm^{-1}). Band-integrated quantities are obtained using the option `output_process per_band`. The sum over all bands can be calculated using the option `output_process sum`.

The example `examples/UVSPEC_REPTRAN_THERMAL.INP` calculates brightness temperatures of band-integrated radiances in the thermal range from different viewing zenith angles at top of atmosphere:

```
rte_solver disort          # Radiative transfer equation solver

# Uncomment the following line to use finer spectral resolution
#mol_abs_param reptran fine


                           # calculate brightness temperature
output_quantity brightness

albedo 0                   # set albedo to 0, emissivity to 1
source thermal             # thermal
wavelength 2500 100000

zout TOA                   # top of atmosphere
                           # looking downward
umu 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0
phi 0

output_user lambda uu

quiet
```

Fig. 3.7 compares the spectral resolutions of REPTRAN and LOWTRAN. The spectral resolutions are equal for LOWTRAN and REPTRAN medium (5 cm^{-1}). However spectral information was "degraded to 20 cm^{-1} resolution for use in LOWTRAN" (Ricchiazzi et al., 1998) with the effect that LOWTRAN spectra are significantly smoother than REPTRAN medium spectra.

Finally, the example `examples/UVSPEC_REPTRAN_CHANNEL_THERMAL.INP` calculates the thermal brightness temperatures of a channel of a MSG satellite centered at λ=3.9μm looking at different viewing zenith angles:

```
include ../examples/UVSPEC_REPTRAN_THERMAL.INP

                     # Satellite channel using representative wavel.
mol_abs_param reptran_channel msg1_seviri_ch039
```

This setup is the same as in the previous input file whereby channel integrals are calculated instead of band integrals (`mol_abs_param reptran` of the included file is overwritten by `mol_abs_param reptran_channel` here). The available channels are listed in `data/correlated_k/reptran/channel_list.txt`.

Though we recommend REPTRAN for spectral calculations, the molecular absorption parameterization from LOWTRAN/SBDART by Ricchiazzi et al. (1998) is available mainly for compatibility reasons. LOWTRAN allows for **pseudo-spectral calculations** in the whole spectral range, the respective section of this paper says:

> SBDART relies on low-resolution band models developed for the LOWTRAN 7 atmospheric trans-mission code (Pierluissi and Peng, 1985). These

> models provide clear-sky atmospheric transmission from 0 to 50000 cm-1 and include the effects of all radiatively active molecular species found in the earth s atmosphere. The models are derived from detailed line-by-line calculations that are degraded to 20 cm-1 resolution for use in LOWTRAN. This translates to a wavelength resolution of about 5 nm in the visible and about 200 nm in the thermal infrared. These band models represent rather large wavelength bands, and the transmission functions do not necessarily follow Beers Law. This means that the fractional transmission through a slab of material depends not only on the slab thickness, but also on the amount of material penetrated before entering the slab. Since the radiative transfer equation solved by SBDART assumes Beers Law behavior, it is necessary to express the transmission as the sum of several exponential functions (Wiscombe and Evans, 1977). SBDART uses a three-term exponential fit, which was also obtained from LOWTRAN 7. Each term in the exponential fit implies a separate solution of the radiation transfer equation. Hence, the RT equation solver only needs to be invoked three times for each spectral increment. This is a great computational economy compared to a higher order fitting polynomial, but it may also be a source of significant error.

The LOWTRAN/SBDART gas parameterization is invoked with `mol_abs_param LOWTRAN`. The spectral resolution may be arbitrarily chosen by the user. If not explicitely defined with `wavelength_grid_file`, an internal grid with a step width of 0.5nm below 350nm and 1nm above 350nm is chosen which is practically overkill for most applications in the infrared. An extraterrestrial spectrum covering the complete solar range is provided at two different resolutions, `data/solar_flux/kurudz_1.0nm.dat` and `data/solar_flux/kurudz_0.1nm.dat`. An example for the solar range is shown in `examples/UVSPEC_LOWTRAN_SOLAR.INP`:

```
atmosphere_file ../data/atmmod/afglus.dat
source solar ../data/solar_flux/kurudz_1.0nm.dat

albedo 0.2               # Surface albedo
sza 30.0                 # Solar zenith angle

rte_solver twostr       # Radiative transfer equation solver
pseudospherical
wavelength 250.0 2500.0  # Wavelength range

mol_abs_param LOWTRAN    # select LOWTRAN molecular absorption

aerosol_default
aerosol_visibility 20

quiet
```

while `examples/UVSPEC_LOWTRAN_THERMAL.INP` shows how to do a thermal calculation:

```
# uvspec data files
data_files_path ../data/
atmosphere_file ../examples/AFGLUS.70KM
source thermal ../examples/UVSPEC_LOWTRAN_THERMAL.TRANS

rte_solver twostr     # Radiative transfer equation solver
pseudospherical
wavelength_grid_file ../examples/UVSPEC_LOWTRAN_THERMAL.TRANS

mol_abs_param LOWTRAN  # select LOWTRAN molecular absorption

output_process per_nm

quiet
```

Please note the following points:

- Thermal radiation is per default output in W/(m^{2}cm^{-1}), if the bandwidth is equal to 1 cm^{-1} (default for `mol_abs_param LOWTRAN` calculations). Otherwise the output is the integrated flux over the wavenumber interval specified by `thermal_bandwidth`, `thermal_bands_file`, or by the `mol_abs_param` option (Kato, Kato2, Kato2.96, Fu, AVHRR_KRATZ, or Generic). To convert e.g. to W/(m2 nm) use `output_process per_nm` or multiply with k/lambda where k is the wavenumber [cm^{-1}] and lambda is the wavelength [nm]. To calculate band-integrated thermal quantities please consider `thermal_bands_file`.
- Even though no extraterrestrial irradiance is required, a `source thermal file` may be specified for the thermal case. The reason is that, as explained initially, the `source thermal file` defines the output grid. The second column in `source thermal file` can be chosen arbitrarily in this case because it is ignored.
- For the choice of the wavelength grid for the calculation (`wavelength_grid_file`) please consider that the resolution of the absorption parameterization is 5 cm^{-1} which translates to 0.3nm at 750 nm and to 50 nm at 10 μm. Choosing higher resolutions for the internal wavelength grid (`wavelength_grid_file`) is usually a waste of computational time.
- Please also make sure to choose a fine enough spectral resolution in order to capture all absorption features.

The red curve in Fig. 3.7 demonstrates the spectral resolution of the LOWTRAN/SBDART absorption parameterization (and REPTRAN, see above) for two selected wavelength intervals of the solar and thermal range. The resolution of LOWTRAN is about 5 cm^{-1} which translates to about 0.3 nm in the left figure (oxygen A-band) and 50nm in the right figure (ozone absorption band in the atmospheric window). Compare this figure to the above line-by-line example to get an impression about the differences between the methods.

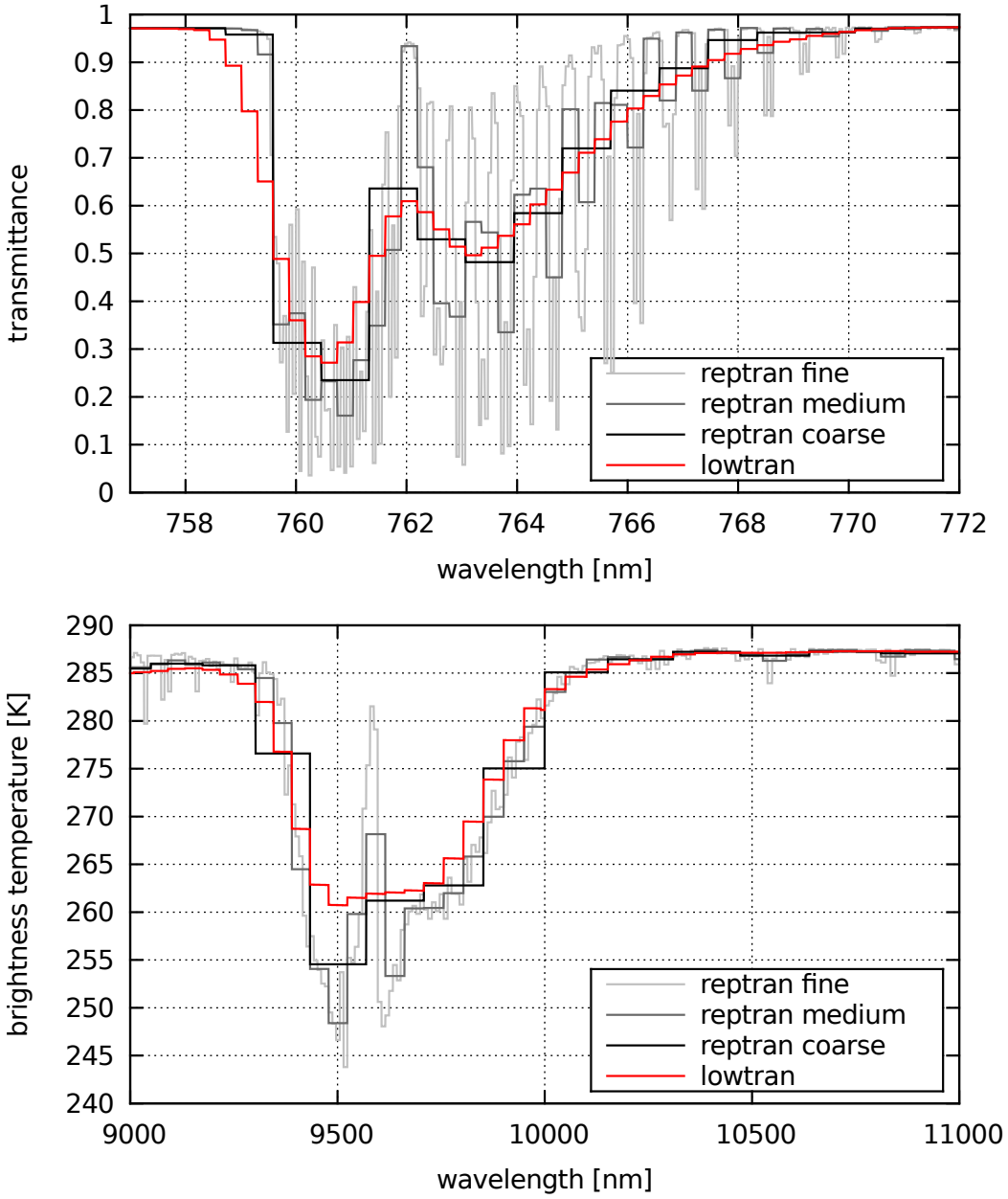

Figure 3.7: Two selected wavelength intervals in the solar range (upper panel, O2A band) and the thermal range (lower panel, O3 band at $\lambda \approx 9.6\mu$m), to demonstrate the spectral resolution of the LOWTRAN and REPTRAN absorption parameterizations.

3.3.3 Surface properties

The most simple way to define the surface properties is to define a Lambertian surface with constant albedo using the option `albedo` or a wavelength dependent surface albedo using `albedo_file`. *libRadtran* provides the spectral surface albedo library of the International Geosphere Biosphere Program (IGBP) which can be selected with `albedo_library IGBP`. It contains 20 surface tpyes such as "mixed forest", "cropland", or "urban" and the tye can be selected using `brdf_surface_type`.

For accurate radiance simulations, the directional dependence of surface reflection should be taken into account by specifying the biderectional reflectance distribution function (BRDF). Note that this works only in combination with the RTE solvers DISORT (`rte_solver disort`) or MYSTIC (`rte_solver mystic`).

For water surfaces it is very important to take into account the directional dependence when the sun-glint is observed, because here the surface reflection becomes very high. The BRDF of water surfaces can be parameterized using the option `brdf_cam` following Cox and Munk (1954a,b) and Nakajima and Tanaka (1983). The respective parameters are the wind speed `brdf_cam u10`, the pigment concentration `brdf_cam pcl`, and the salinity `brdf_cam sal`. Further, the model developed by Tsang et al. (1985), which takes into account shadowing by surface waves, is available (`bpdf_tsang_u10`). Both models can be used for simulations with and without polarization.

Various BRDF parameterizations for land surfaces are included in *libRadtran*. The AMBRALS parameterization (option `brdf_ambrals` is based on the semiempirical Ross-Li (reciprocal RossThick-LiSparse) model and requires the three parameters f_{iso}, f_{vol} and f_{geo} (see Eq. 37 in Lucht et al. (2000) for the defintions). In order to include the spectral dependence of these parameters the option `brdf_ambrals_file` is available. Another implemented BRDF model for land surfaces is the RPV paramterization (Rahman et al., 1993b; Degünther and Meerkötter, 2000) which may be selected using the option `brdf_rpv`. For this model, *libRadtran* provides pre-calcualted data for 17 surface types defined by the International Geosphere-Biosphere Program (IGBP) (`brdf_rpv_library IGBP`). The surface type of the library can be selected with `brdf_rpv_type`. For simulations with polarization two bidirectional polarized reflectance function (BPDF) models are available: `bpdf_litvinov` (Litvinov et al., 2012) and `bpdf_maignan` (Maignan et al., 2009). These combine BPDF models with the Fresnel surface reflection matrix.

Complete descriptions of all parameters of the BRDF/BPDF models are given in section 6.1 and in the corresponding reference publications.

3.3.4 Aerosol

All options to set up and modify aerosol properties start with `aerosol_`. Aerosols may be specified in a hierarchical way. The most simple way to define an aerosol is by the command `aerosol_default` which will set up the aerosol model by Shettle (1989). The default properties are a rural type aerosol in the boundary layer, background aerosol above 2km, spring-summer conditions and a visibility of 50km. These settings may be modified with `aerosol_haze`, `aerosol_vulcan`, `aerosol_season`,

and `aerosol_visibility`. More information can be introduced step by step, overwriting the default parameters. `aerosol_file tau`, `aerosol_file ssa`, and `aerosol_file gg`, can be used to define the profiles of optical thickness, single scattering albedo, and asymmetry parameter. The integrated optical thickness can be set to a constant value using `aerosol_modify tau set` or scaled with `aerosol_modify tau scale`. The single scattering albedo may be scaled by `aerosol_modify ssa scale` or set to a constant value by `aerosol_modify ssa set`. The aerosol asymmetry factor may be set by `aerosol_modify gg set`. The wavelength dependence of the aerosol optical depth is specified using the `aerosol_angstrom` parameter. `aerosol_file moments` allows specification of the scattering phase function. If microphysical properties are available these may be introduced by defining the complex index of refraction `aerosol_refrac_index` and the size distribution `aerosol_sizedist_file`. Finally, one may define the aerosol optical properties of each layer explicitely using `aerosol_file explicit`.

The following list is an overview of some aerosol description parameters. The entries are arranged in a way that a parameter 'overwrites' all values higher up in the list.

aerosol_default
: Generate default aerosol according to Shettle (1989).

aerosol_vulcan, aerosol_haze, aerosol_season, aerosol_visibility
: Set Shettle (1989) aerosol properties (aerosol type, visibility)

aerosol_file explicit
: Specify optical properties of each layer explicitly, that is, extinction coefficient, single scattering albedo, and the moments of the phase function (everything as a function of wavelength).

aerosol_file tau , aerosol_file ssa, aerosol_file gg
: Overwrite profiles of optical thickness, single scattering albedo, and asymmetry parameter

aerosol_file moments
: Specify a phase function to be used instead of the Henyey-Greenstein phase function

aerosol_refrac_index, aerosol_sizedist_file
: Calculate optical properties from size distribution and index of refraction using Mie theory. Here is an exception from the rule that ALL values defined above are overwritten because the optical thickness profile is re-scaled so that the optical thickness at the first internal wavelength is unchanged. It is done that way to give the user an easy means of specifying the optical thickness at a given wavelength.

aerosol_species_file
: Define profiles of arbitrary aerosol types. The profiles will be mixed within *uvspec*. Optical properties of the aerosol types can be provided using the option `aerosol_species_library`. One library may be downloaded from `www.libradtran.org`, it inlcudes aerosol optical properties based on size distribution parameters and refractive indices from the OPAC database (Hess et al., 1998). The

optical properties have been generated using the `mie` tool and they include full phase matrices, e.g. they are suitable for calculations with polarization.

aerosol_modify gg/ssa/tau scale/set
Overwrite profiles of asymmetry parameter and single scattering albedo

aerosol_angstrom
Overwrite the integrated optical thickness (profiles are not changed).

An example for a *uvspec* aerosol description is

```
include ../examples/UVSPEC_CLEAR.INP

aerosol_vulcan 1               # Aerosol type above 2km
aerosol_haze 6                 # Aerosol type below 2km
aerosol_season 1               # Summer season
aerosol_visibility 20.0        # Visibility
aerosol_angstrom 1.1 0.2       # Scale aerosol optical depth
                               # using Angstrom alpha and beta
                               # coefficients
aerosol_modify ssa scale 0.85  # Scale the single scattering albedo
                               # for all wavelengths
aerosol_modify gg set 0.70     # Set the asymmetry factor
aerosol_file tau ../examples/AERO_TAU.DAT
                               # File with aerosol optical depth profile
```

By combining this with the clear sky example given above a complete *uvspec* input file including aerosol is constructed.

3.3.5 Water clouds

All options to set up and modify water cloud properties start with `wc_`.

The easiest way to define a water cloud is to specify a `wc_file` which defines the liquid water content and effective droplet radius at each model layer or level. By combining the following lines with the clear sky example given above a complete *uvspec* input file including water clouds is constructed.

```
include ../examples/UVSPEC_CLEAR.INP

wc_file 1D ../examples/WCSIMPLE.DAT # Location of water cloud file
wc_modify tau set 15.               # Set total water cloud optical depth
```

A typical example for a wc_file looks like:

```
# z LWC R_eff
# (km) (g/m3) (um)
5.000 0 0
4.000 0.2 12.0
3.000 0.1 10.0
2.000 0.1 8.0
```

The three columns are the level altitude [km], the liquid water content [g/m^3], and the effective droplet radius [micrometer]. Per default (since version 1.4), these quantities are interpreted as layer quantities, and in the above example, the cloud would extend from 2 to 5 km, with e.g. a LWC of 0.2 g/m^3 for the layer between 4 and 5 km. Before version 1.4 the `wc_file` was interpreted as level quantities (unless `wc_layer` was specified). That is, the value 0.2 g/m^3 referred to altitude 4.0 km, as e.g. in a radiosonde profile. The properties of each layer were calculated as average over the adjacent levels. E.g. the single scattering properties for the model layer between 3 and 4 km were obtained by averaging over the two levels 3 km and 4 km. To allow definition of sharp cloud boundaries, clouds were only formed if both liquid water contents above and below the respective layer were larger than 0. Hence, in the above example, the layers between 2 and 3 as well as between 3 and 4 km were cloudy while those between 1 and 2km and between 4 and 5 km were not. To switch to the old behaviour, use `interpret_as_level wc`.

To make sure that the clouds really look as you want them to look, it is recommended to use the `verbose` option. This option shows not only where the cloud is actually placed, it rather tells the user exactly how LWC and effective radius are translated into optical properties, depending on the choice of parameterisation. Please also note that the definition of the empty top level at 5km is important to tell *uvspec* where the cloud ends. If omitted, the cloud would extend all the way to the top of the atmosphere.

There are different ways to convert the microphysical properties to optical properties. Either a parameterization is used, like the one by Hu and Stamnes (1993) (which is the default), or by Mie calculations. The latter are very time-consuming, hence we decided not to include these online into *uvspec* but rather have an option to read in pre-calculated Mie tables. The option `wc_properties` controls the method: `hu` selects the Hu and Stamnes (1993) parameterization, `mie` selects pre-calculated Mie tables which are available at `http://www.libradtran.org`. The tables include the full scattering phase matrices and can therefore be used for polarization dependent calculations. If `wc_properties mie` is selected, the model expects one or more Mie cloud property files including each internal wavelength which is useful for the fixed wavelength grids used by the correlated-k parameterisations `mol_abs_param kato`, `mol_abs_param fu`, etc. For a spectral calculation with free wavelength grid, there is also the possibility to use a pre-defined set of Mie tables (available at the web site) and to define `wc_properties mie interpolate` to automatically interpolate the Mie properties to the internal wavelength grid. Although this is an extremely useful option, please use it careful because it might consume enourmous amounts of memory. Finally, there is the option to define an arbitrary file which can be generated using the `mie` tool (see section 4).

As for the aerosol, there are several options to modify the optical properties of the clouds. And of course there is also the option of defining all cloud properties explicitely using `wc_file moments`.

3.3.6 Ice clouds

Ice clouds are generated in a similar way to water clouds. All options to set up and modify ice cloud properties start with `ic_`. The main difference between water and ice clouds is

that the latter usually consist of non-spherical particles. Hence, the conversion from microphysical to optical properties is much less defined, and several parameterizations are available. Please note in addition that there are different definitions of the effective radius. E.g. the parameterizations by Key et al. (2002) and Baum et al. (2005b, 2007) use the same definition whereas Fu (1996) actually uses another definition (see explanation of `ic_properties`). Finally, the sharp forward peak which is typical for ice particles can also be treated differently: E.g., Fu (1996) provides delta-scaled optical properties while Key et al. (2002) uses unscaled parameters (see explanation of `ic_fu deltascaling`). Figure 3.8 illustrates the implications. Plotted are extinction coefficient, asymmetry parameter, and single scattering albedo for ice clouds with an effective radius of 25 micrometers as a function of wavelength. If treated consistently, all parameterizations Key et al. (2002), Fu (1996), and Baum et al. (2005b, 2007) provide nearly identical results (solid lines, default settings in *uvspec*). If the definition of effective radius by Fu (1996) and delta-scaling is applied the optical properties look different. The effect of delta scaling on a radiative transfer calculation is that the direct irradiance in increased and the diffuse irradiance is decreased, whereas the global irradiance remains unchanged. The definition of the effective radius has a smaller effect but it modifies also the global irradiance. Note that the parameterization by Baum et al. (2005b, 2007) is plotted only up to 2200 nm. The reason is that it does not cover the full spectral region, it is available for two spectral regions (from 0.4–2.2 μm and from about 3–100 μm). For the calculation of radiances one should use either `ic_properties baum`, `hey`, `baum_v36` or `yang2013` because these parameterizations include complete scattering phase functions and do not use approximations like the Heney-Greenstein phase function. `hey`, `baum_v36` and `yang2013` can also be used for polarized radiative transfer. The data needed for `baum`, `hey`, `baum_v36`, and `yang2013` is available at `www.libradtran.org`.

3.3.7 Calculation of radiances

To calculate radiances the following lines will do the job when combined with the clear sky example above

```
include ../examples/UVSPEC_AEROSOL.INP # Include's may be nested.

rte_solver disort  # This override what is specified in above file
                   # and files included in that file etc.

phi0 40.0          # Solar azimuth angle
umu  -1.0 -0.5  -0.2 -0.1             # Output cosine of polar angle
phi 0.0 45. 90. 135. 180.0 225. 270.0 # Output azimuth angles
```

In this example radiances are calculated for the specified directions, where `umu` are the cosines of the viewing zenith directions and `phi` are the viewing azimuth angles.

The following examples shows a complete input file for the calculation of polarized radiances using MYSTIC:

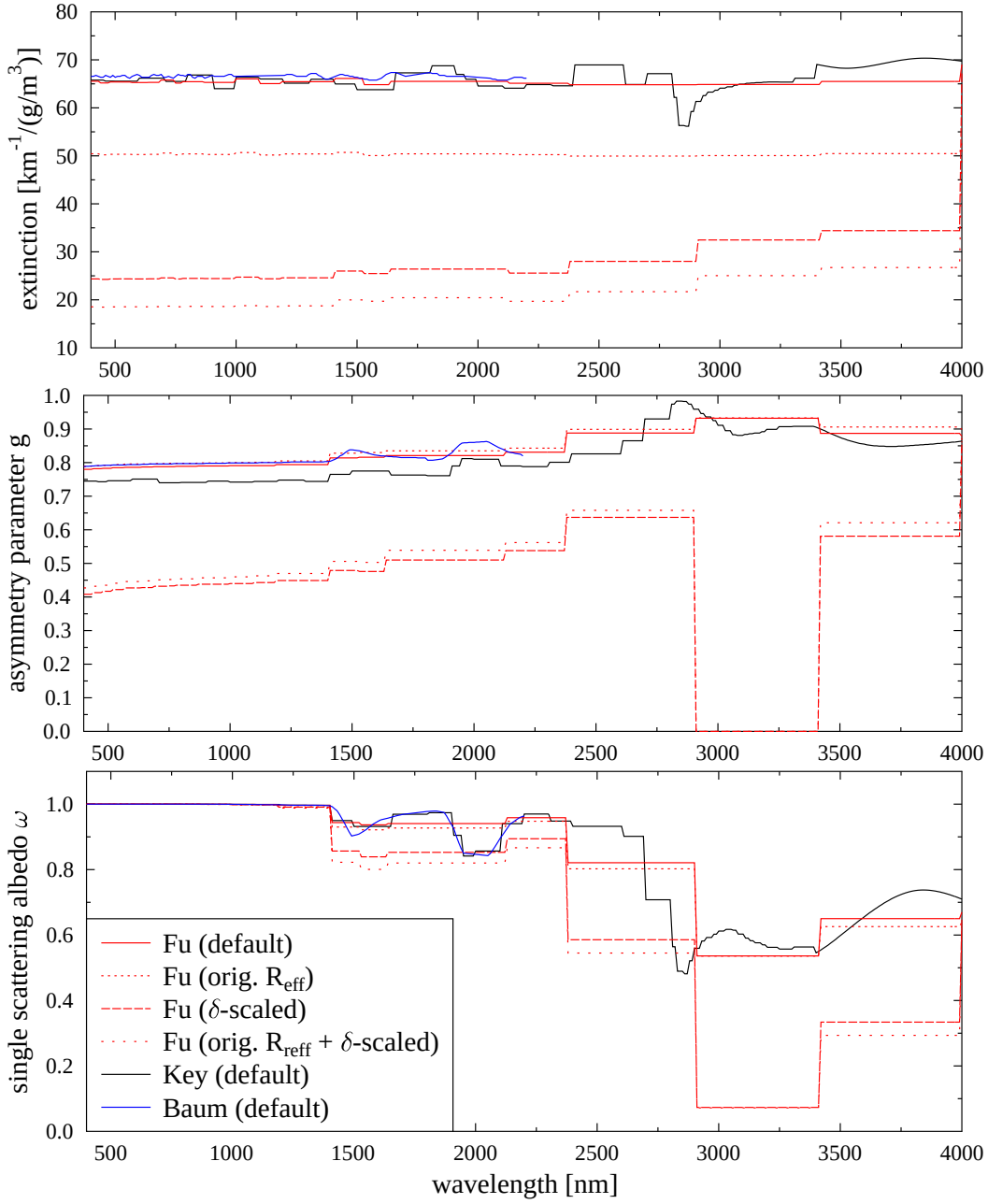

Figure 3.8: Extinction coefficient, asymmetry parameter, and single scattering albedo for ice clouds with an effective radius of 25 μm as a function of wavelength for various parameterizations.

```
                          # Location of atmospheric profile file.
atmosphere_file ../examples/UVSPEC_MC_ATM.DAT
                          # Location of the extraterrestrial spectrum
source solar ../data/solar_flux/atlas_plus_modtran
mol_modify O3 300. DU
day_of_year 170           # Correct for Earth-Sun distance
albedo 0.2                # Surface albedo
sza 30.0                  # Solar zenith angle
phi0 180.0                # Sun in the North

rte_solver montecarlo     # Radiative transfer equation solver MYSTIC
mc_photons 1.e6            # MYSTIC number of photons

mc_polarisation
wavelength 310.0          # Wavelengths considered

umu -0.5                  # Viewing direction
phi 40

quiet

# The results given in UVSPEC_MC_POL.OUT can be found in the file
# mc.rad, columns 3,4,8.
# Column 3 and 4 are the viewing zenith and azimuth and column 8 is the
# Stokes vector (I,Q,U,V).
# For routine applications please use mc.rad.spc instead.
```

This example is only for a 1D clear sky atmosphere. For radiance calculations it is strongly recommended to use the local estimate method (`mc_escape`, e.g. Marshak and Davis (2005)) which significantly reduces the noise in the results. Further, for radiance calculations in the presence of clouds or any other particle type with strong forward scattering peak, we strongly recommend to use the variance reduction technique VROOM (`mc_vroom`, Buras and Mayer (2011)).

Chapter 4

Calculation of optical properties - `mie`

libRadtran includes the tool `mie` to calculate optical properties of spherical particles. Two different efficient and well tested Mie codes are implemented: The one by Wiscombe (1980) and the one by Bohren and Huffman (1998). Scattering phase matrices and corresponding Legendre polynomials can currently only be calculated using the code by Wiscombe (1980).

4.1 Basic usage

4.1.1 Running `mie`

Mie scattering calculations are performed for a specified wavelength interval. The `mie` program reads input from standard input, and outputs to standard output or to a file. If `output_user netcdf` is specified `mie` generates a file that can be used for radiative transfer calculations with `uvspec`.

The `mie` tool is normally invoked in the following way:

```
mie < input_file > output_file
```

Warning: Please note the error checking on input variables is very scarce at the moment. Hence, if you provide erroneous input, the outcome is unpredictable.

4.1.2 The `mie` input file

The `mie` input file consists of single line entries, each making up a complete input to the mie program. First on the line comes the parameter name, followed by one or more parameter values. The parameter name and the parameter values are seperated by white space.

Filenames are entered without any surrounding single or double quotes.

Comments are introduced by a `#`. Blank lines are ignored.

4.1.3 Model output

The standard output (stdout) of the mie program is one line for each wavelength and each effective radius. The format of the output line is

```
  lambda refrac_real refrac_imag qext omega gg spike pmom
```

For the meaning of the keywords please refer to the description of input option `output_user`. The Legendre polynomials `pmom` are only caclulated if the option `nmom` is specified.

If `output_user netcdf` is specified the output is written to a netcdf file in the format that is required by `uvspec`.

4.2 Examples

4.2.1 Calculation for one particle

The following example shows a Mie calculation for a single spherical particel with a radius of 200 μm. The refractive index is specified by the user. The calculation is performed for wavelengths from 280 to 5000 nm in 5 nm steps.

```
mie_program MIEV0              # Select Mie code by Wiscombe
refrac user 1.75  0.16         # Specify refractive index
r_eff 200.                     # Specify particle radius
wavelength  280. 5000.         # Define wavelengths
wavelength_step 5.
```

4.2.2 Calculation for a size distribution

Not all cloud droplets are of one specific size. The cloud droplet size spectrum may be represented for instance by a gamma distribution. Gamma distributions can easily be specified using the option `distribution gamma` as demonstrated in the following example:

```
mie_program MIEV0            # Select Mie code by Wiscombe
refrac water                 # Use refractive index of water
r_eff 4 12 1                 # Specify effective radius grid
distribution gamma 7         # Specify gamma size distribution (alpha=7)
wavelength  1600 1600        # Define wavelength
nstokes 4                    # Calculate all phase matrix elements
nmom 500                     # Number of Legendre terms to be computed
nmom_netcdf 129              # Number of Legendre terms to be stored in
                             #    netcdf file, must be > number_of_streams
nthetamax 500                # Maximum number of scattering angles to be
                             #    used to store the phase matrix
output_user netcdf           # Write output to netcdf file
verbose                      # Print verbose output
```

The refractive index of water is taken for this calculation. In order to generate input for `uvspec` Legendre polynomials and from those the phase matrices need to be calculated. The option `nmom` specifies how many Legendre polynomials shall be computed. If the selected number is too small for an accurate representation of the phase matrix, a warning is given. If `output_user netcdf` is specified the corresponding phase matrices are calculated from the Legendre moments. The scattering angle grid is optimized so that the phase matrix is sampled as accurate as possible. The option `nthetamax` can be used to set an upper limit of scattering angle grid points to be used. This example generates a netcdf file which can directly be used in `uvspec` with the options `wc_properties` or `ic_properties`.

Chapter 5

Further tools

Besides *uvspec* and *mie libRadtran* provides several small tools related to radiative transfer in the atmosphere. These tools can be found in the `bin` directory. Some of the tools are described in this chapter.

Help for all tools can be obtained on the command line using the option `-h`.

5.1 General tools

5.1.1 Integration - `integrate`

`integrate` calculates the integral between limits $x_{\min}$ and $x_{\max}$ by interpolating the data points (x[i], y[i]) with natural cubic splines or linear interpolation. $x_{\min}$ and $x_{\max}$ are the minimum and maximum values of the first column in the input file. The x-values in the first column must be in ascending order.

The different options to `integrate` are displayed when executing:

```
integrate -h
```

5.1.2 Interpolation - `spline`

`spline` interpolates discrete data points using natural cubic splines or linear interpolation. The x-values in the first column must be in ascending order.

The different options to `spline` are displayed when executing:

```
spline -h
```

5.1.3 Convolution - `conv`

`conv` convolutes a spectrum with a given filter function.

The different options to `conv` are displayed when executing:

```
conv -h
```

5.1.4 Add level to profile - `addlevel`

`addlevel` is a simple shell script to add a level to an atmosphere_file or mol_file. It is located in the `src` directory.

The different options to `addlevel` are displayed when executing:

```
addlevel -h
```

5.1.5 Numerical difference between two files -`ndiff`

The Perl script `ndiff` calculates the relative difference between two files containing columns of numbers (file1/file0). The first column is not included. The calculated differences are output to stdout. If limit is different from 0.0, the number of differences greater than abs(maxdiff) are printed to stdout. The `ndiff` script is extensively used by the `test/test.pl` script invoked by `make check`.

The `ndiff` script is invoked by

```
ndiff [options] file0 file1
```

The script understands the following options

–limit <**value**> The minimum value in file0 considered when counting the number of differences between file0 and file1. Default is 0.0.

–maxdiff <**value**> The maximum relative difference allowed between file0 and file1. Defaut is 0.0.

–sub Subtract file1 - file0 instead of division

–nox First column is included

–quiet The differences are not output, but the number of differences are still printed.

–help Print help message.

5.2 Tools to generate input data to and analyse output data from `uvspec`

5.2.1 Calculate albedo of snow - `Gen_snow_tab`, `snowalbedo`

The `Gen_snow_tab.pl` script and the `snowalbedo` program may be used to calculate the diffuse and direct albedo of snow as formulated by Warren and Wiscombe (1980).

First a table of various snow optical properties must be generated. This is done by the PerlGen_snow_tab.pl script. The resulting tables will be read by the snowalbedo program which will calculate the wanted surface albedo quantities.

Generating the tables by the Gen_snow_tab.pl script is straightforward as the script only takes one argument, namely the name of the file body (It will also print a small help message if -help is given to it). The script will generate three files with extensions .gg, .qext and .ssa.

```
perl Gen_snow_tab.pl --file <name>
```

The generated tables is read by the snowalbedo program which requires the following options:

-l Equivalent depth of liquid water in snowpack (g cm -2)

-r mean grain radius (μm)

-u cosine of solar zenith angle

The options below are optional

-a albedo of underlying surface, default 0.03

-p turn of printing of messages

-h Print help message.

A typical usage of snowalbedo is (Gen_snow_tab.pl -file ../examples/MIE_ICE_TAB has been executed first)

```
snowalbedo ../examples/MIE_ICE_TAB -l 0.05 -r 50 -u 0.5 -p
```

This will produce the following output (only two first output lines shown)

```
290.0 2.00893  0.9999776000 0.88037   0.9728   0.9689
291.0 2.01212  0.9999782400 0.88064   0.9731   0.9693
```

Here, the various columns have the following content

1. wavelength (nm)
2. Q_ext
3. Single scattering albedo
4. Asymmetry parameter
5. Direct albedo
6. Diffuse albedo

5.2.2 Calculate cloud properties - `cldprp`

`cldprp` calculates wavelength-dependent cloud properties using one of several parameterizations.

The different options to `cldprp` are displayed when executing:

```
cldprp -h
```

5.2.3 Solar zenith and azimuth angle - `zenith`

The `zenith` tool calculates the solar zenith and azimuth angle for a given time and location. Output is to stdout and is self-explanatory (unless the `-q` option is used).

The solar zenith and azimuth angles are calculated using the algorithm of Blanco-Muriel et al. (2001). If the `-S` option is invoked the Spencer (1971) algorithm is used.

The `zenith` tool is invoked by

```
zenith [options] <day> <month> <hour> <min> [sec]
```

where the various options are

-a <latitude> Latitude (North positive)

-o <longitude> Longitude (West positive)

-s <std. long> Standard Longitude (West positive) this is the longitude to which the time zone refers (-15 deg for central Europe, corresponds to UTC+1).

-l <location> Instead of `-a`, `-o` and `-s` define a location. possible locations are mim, ifu, dlrop.

-y <yyyy> year; not used if -S specified, default: 2003.

-S Use the Spencer algorithm.

-e Calculate eccentricity.

-t <UTC + x> Time zone; e.g. -t2 means UTC + 2.

-q Be quiet.

-h Print help message.

The options below apply if the solar zenith angle is wanted as a function of wavelength. This is useful for simulation of scanning spectroradiometer measurements. Output is two columns with wavelength and solar zenith angle. All options must be specfied. However <hour> and <min> should not be specified. To avoid too much output use the `-q` option.

-B start_time (decimal hours of Greenwich time)

-E end_time (decimal hours of Greenwich time)

-u start_wavelength (nanometers)

-v end_wavelength (nanometers)

-w step_wavelength (nanometers)

The following invocation of `zenith` calculates the solar zenith and azimuth angles at the time and location of the writing of this text

```
zenith -a 62.462052 -o -6.303358 -s -15 -y 2010 4 3 9 35
```

5.2.4 Local noon time - `noon`

The `noon` tool calculates the local noon time given a location in terms of longitude and latitude or a location name using the `-l` option. Output is to stdout and is self-explanatory.

The local noon time is calculated using the algorithm of Blanco-Muriel et al. (2001). If the `-S` option is invoked the Spencer (1971) algorithm is used.

The `noon` tool is invoked by

```
noon [options] <day> <month>
```

where the various options are

-a <latitude> Latitude (North positive)

-o <longitude> Longitude (West positive)

-s <std. long> Standard Longitude (West positive) this is the longitude to which the time zone refers (-15 deg for central Europe, corresponds to UTC+1).

-l <location> Instead of `-a`, `-o` and `-s` define a location. possible locations are ifu, dlrop.

-y <yyyy> year; not used if -S specified, default: 2003.

-S Use the Spencer algorithm.

-h Print help message.

The following invocation of `noon` calculates the noon time at the home location of one of the *libRadtran* developers for his wedding date.

```
noon -a 62.462052 -o -6.303358 -s -15 -y 1992 29 2
```

5.2.5 Angular response and tilted surfaces - `angres`

The `angres` tool takes a precalculated radiance field and integrates it over a given angular area using any angular response. Typical usages of `angres` are calculation of radiation on tilted surfaces and estimation of effects of imperfect angular response functions.

The `angres` tool is invoked as follows:

```
angres angres_file raddis_file
```

The two required input files will be read by the `angres` tool.

angres_file is a two column file with the first column holding the angle and the second column the angular response, e.g. a measured cosine response. To generate standard angular response function see the `make_angres_func` tool.

raddis_file holds the radiance distribution as output from uvspec with the disort solvers for one single wavelength.

After reading the two input files the angular response will be tilted and rotated if specified with the `-t` and `-r` options respectively. Finally the product of the resulting angular response and radiance distribution field are integrated using Monte Carlo methods to yield the effective response. The integration is done for the diffuse radiation field only. To include the direct contribution the -s and -z options must be set to give the direction of the sun.

Output is 3 numbers:

1. The integral of the diffuse radiation field times angular response.
2. Estimated absolute error of the above integral.
3. The integral of the diffuse+direct radiation field times angular response (requires that `-s` and `-z` are specified, otherwise same as first number

The angles in the `angres_file` must be in radians if not the `-a` option is used. The `raddis_file` must contain output from `uvspec` run for one single wavelength with one of the disort solvers and with `phi` and `umu` set. Note that the angles in the `angres_file` must follow the same conventions as for the disort algorithm. This is different from that typically used when reporting measurements of the angular response.

The `angres` tool accepts the following command line options:

-h show this page.

-c number of random points used for Monte Carlo integration.

-i The diffuse radiation is assumed to be isotropic.

-a angular response angle given in degrees and not cosine of angle.

-r rotation angle in degrees.

-t tilt angle in degrees.

-s solar zenith angle in degrees.

-z solar azimuth angle in degrees.

-p pgm files are made of the angular response before and after tilt and rotate.

Sample `angres` input and output files are found in the `examples` directory. The following

```
angres examples/ANGRES_1_ANG.DAT  \
       examples/ANGRES_RADDIS_1.DAT -a -t -r 0 -s 32 -z 0
```

calculates the radiation on a horisontal surface given the angular response in `examples/ANGRES_1_ANG.DAT`. The input used to calculate the radiance file is given in the start of `examples/ANGRES_RADDIS_1.DAT`.

An example of the use of `angres` together with `uvspec` is given in Mayer and Kylling (2005, section 4.6).

5.2.6 Angular response function - `make_angresfunc`

The `make_angresfunc` tool calculates various angular response functions to be used by for example the `angres` tool. All output is to stdout in two column format. The first column is the angle and the second column contains the corresponding value for a given angular response. The output angles follow `disort` conventions.

The `make_angresfunc` tool is invoked on the command line as

```
    make_angresfunc [-hart]
```

where the various options are

-t type of angular response

1. cosine (default)
2. 2pi actinic flux
3. 4pi actinic flux

-a angular output format

1. angles (default)
2. cosine of angle

-r resolution, in degrees

-h Print help message.

The following invocation of `make_angresfunc` calculates the angular response for a perfect cosine detector. The output is found in the `examples/ANGRES_1_ANG.DAT`.

```
make_angresfunc -t 1 -r 1
```

5.2.7 Slit function generator - `make_slitfunction`

To generate standard slit functions to be used by `uvspec` the `make_slitfunction` tool may be used. For a given set of input it outputs to stdout in two column format the wavelength and corresponding value for the wanted slit function.

The `make_slitfunction` tool is invoked on the command line as

```
make_angresfunc [-hrtf]
```

where the various options are

-t type of slitfunction

1. triangular (default)
2. rectangular
3. Gaussian

-f full width at half maximum, in nm

-r resolution, in nm

-n number of fwhm (in nm) spanned by the slit function. Only applicable with Gaussian (type 3) slit function. Default value is 4.

-h Print help message.

The following invocation of `make_slitfunction` calculates the a triangular slit function with FWHM of 0.75 nm and a resolution of 0.01 nm. The output is found in the `examples/TRI_SLIT.DAT`.

```
make_slitfunction -f 0.75 -r 0.01 -t 1
```

5.2.8 Calculate phase function from Legendre polynomials - `phase`

The `phase` tool takes a Legendre series as input and calculates the corresponding phase function.

The program is invoked as follows:

```
phase [options] <filename>
```

The following optional arguments may be specified:

-h Display help message.

-c 1-column input.

-b Binary (netcdf) input.

-d Use scattering angle in degrees instead of the cosine of the scattering angle μ.

-s <**step**> Step width for evaluation (default: 0.01).

-o <number of digits> Optimize scattering angle grid.

-x <**filename**> File containing μ-values to be interpolated.

-n Normalize phase function.

-f Use delta scaling.

The format of the input file is as generated by the `mie` program. the first 7 columns are ignored, the following columns are assumed to hold the moments of the phase function. If option `-c` is specified, the input file is considered a one column file holding one moment per line.

5.2.9 Perform Legendre decomposition of phase function - `pmom`

The `pmom` tool calculates the Legendre moments of a given phase function. The input must be provided as 2-column file, containing the scattering angle grid in the first column and the phase function value in the second column. The output of `pmom` are the Legendre moments.

The `pmom` tool is invoked on the command for instance as

```
pmom [options] <filename>
```

The following optional arguments may be specified:

-h Display help message.

-l <**number**> Number of Legendre moments to be computed. In order to obtain an accurate decomposition of the phase function, the last terms of the Legendre series should approach 0.

-r <**grid**> Specify scattering angle grid which is used internally (see below for more explanation).

-c Calculate coefficients instead of polynomials (these include the factor $(2l+1)$. `uvspec` requires Legendre coefficients.

-n Normalize the phase function before computing the Legendre moments.

You may specify the number of moments using the option `-l`. Different scattering angle grid resolutions can be chosen using the option `-r`. For moderate forward peaks, the standard grid (`-r 1` - equidistant, 0.01 degrees step width) should be sufficient. For phase functions with a very strong forward peak, e.g. ice particle phase functions, the finest grid resolution (`-r 2` - equidistant, 0.001 degrees step width) should be specified. If the grid of the input file should be used for the Legendre decomposition, please use `-r 3`; this option uses the new speedy and exact method for Legendre decomposition (Buras, Dowling, Emde 201X). Default. You may test `-r 4` and `-r 5`, in this case non-equdistant grids with a finer resolution around the forward peak are used.

You may test the accuracy of the Legendre decomposition by using the tool `phase`:

```
phase -c -d -s 1 pmom_outfile.dat
```

5.3 Other useful tools

5.3.1 Stamnes tables for ozone and cloud optical depth

Stamnes et al. (1991) devised a method to derive the total ozone column and cloud optical depth from global irradiance measurements. For ozone column retrieval this method requires a table of irradiance ratios as a function of solar zenith angle and ozone column. The irradiance ratio is taken as the ratio of irradiances at non-absorbing and ozone-absorbing wavelengths. The cloud optical depth is retrieved from tables of cloud/cloudless irradiance ratios as a function of solar zenith angle and water cloud optical depth.

The *libRadtran* package comes with three tools for calculation and reading of these so-called Stamnes tables. The Perl script `Gen_o3_tab.pl` is used to generate a matrix of ozone values for solar zenith angle versus a chosen ratio of global irradiances at different wavelengths. For cloud optical depths the Perl script `Gen_wc_tab.pl` may be used to generate a matrix of cloud optical depth for solar zenith angle versus a chosen global irradiance at a selected wavelength. Both tables may be read by the C program `read_Stamnes_tab` which, for a solar zenith angle and a measured ratio, returns the overhead ozone column or cloud optical depth. The Perl scripts `Gen_o3_tab.pl` and `Gen_wc_tab.pl` and the C program are briefly described below. For example of their use please see Mayer et al. (1998); Kylling et al. (2005); Mayer and Kylling (2005).

Generation of the Stamnes ozone column table- `Gen_o3_tab`

The Perl script `Gen_o3_tab.pl` is used to generate a matrix of ozone values for solar zenith angle versus a chosen ratio of global irradiance at different wavelengths. The table is read by the C program `read_Stamnes_tab` which, for a solar zenith angle and a

measured irradiance ratio, returns the overhead ozone column. The following options are understood by `Gen_o3_tab.pl`:

–absolute The wavelengths in the bandpass files are in absolute units. Default is relative units.

–albedo <**value**> Lambertian surface albedo. Default is 0.0.

–alpha <**value**> Angstrom alpha coefficient. Default is 0.0.

–beta <**value**> Angstrom beta coefficient. Default is 0.0.

–altitude <**value**> Altitude above sea level [km]. Default is 0.0.

–atmmod <**name**> Name of atmosphere file. Default atmmod/afglus.dat.

–help Prints help message.

–o3_crs <**name**> Name of o3 cross section to use. Default is Molina. See `uvspec` documentation for other options.

–slitfunction <**name**> Name of slitfunction file.

–bandpasslower <**name**> Name of file holding bandpass for lower wavelength.

–bandpassupper <**name**> Name of file holding bandpass for upper wavelength.

–file <**name**> Name of file where the table will be stored.

–lower_lambda <**value**> Value for lower wavelength, in nm.

–upper_lambda <**value**> Value for upper wavelength, in nm.

–zenith Calculate zenith sky radiance table.

Two different types of tables may be generated depending on the measurement type and the preferred analysis method.

Simple wavelength ratios with `Gen_o3_tab` The simplest type of table is made of ratios of the global irradiance at two single wavelengths. This is the type of table described by Stamnes et al. (1991) and it is typically used to analyse measurements of the global irradiance from spectroradiometers. It is generated by the following command (is line continuation character)

```
perl Gen_o3_tab.pl --slitfunction slitfncfile --lower_lambda 305. \
--upper_lambda 340. --file table.dat
```

Here `slitfncfile` is the name of the slit function file. It is a two column file where the first column is the wavelength (nm, in relative units) and the second column holds the slit function. The slit function must be normalized to unity at the center wavelength.

The generated table `table.dat` is read by `read_Stamnes_tab` for a measured ratio, `-r 10.0`, and solar zenith angle, `-s 30.0`, corresponding to the modelled ratio in the table

```
read_Stamnes_tab -r 10.0 -s 30.0 table.dat
```

Bandpassed wavelength ratios with `Gen_o3_tab` Instead of using single wavelengths it may be of advantage to use ratios of irradiances covering a certain wavelength range and weighted with a bandpass function. This approach may reduce problems due to changes in cloud cover and experimental uncertainties. This approach is also suitable to calculate ozone columns from multichannel, moderate bandwidth filter instruments (Dahlback, 1996). Such tables are generated by

```
perl Gen_o3_tab.pl --slitfunction slitfncfile  --lower_lambda 305.0 \
                   --upper_lambda 320.0 --file table.dat \
                   --bandpasslower bplow.dat --bandpassupper bpupp.dat
```

Here `bplow.dat` and `bpupp.dat` are the bandpass function of the lower and upper wavelength region respectively. The bandpass files have two columns. The first column is the wavelength in nm and relative units to `-lower_lambda` and `-upper_lambda`. If absolute units are specified as for filter instruments, use the `-absolute option`. The second column is the bandpass function.

The tables are read in the same way as the simple wavelength ratio tables.

Generation of the Stamnes cloud optical thickness table - `Gen_wc_tab`

The Perl script `Gen_wc_tab.pl` is used to generate a matrix of cloud optical depth for solar zenith angle versus a chosen global irradiance at a selected wavelength. The wavelength should be chosen such that it is not affected by ozone, e.g. 380 nm. The table is read by the C program `read_Stamnes_tab` which, for a solar zenith angle and a measured irradiance, returns the overhead cloud optical depth. The available options are

–absolute The wavelengths in the bandpass file are in absolute units. Default is relative units.

–albedo <**value**> Lambertian surface albedo. Default is 0.0.

–alpha <**value**> Angstrom alpha coefficient. Default is 0.0.

–beta <**value**> Angstrom beta coefficient. Default is 0.0.

–altitude <**value**> Altitude above sea level [km]. Default is 0.0.

–atmmod <**name**> Name of atmosphere file. Default atmmod/afglus.dat.

–help Prints help message.

–o3_crs <**name**> Name of o3 cross section to use. Default is Molina. See `uvspec` documentation for other options.

–slitfunction <**name**> Name of slitfunction file.

–bandpass <**name**> Name of file holding bandpass for chosen wavelength.

–file <**name**> Name of file where the table will be stored.

–lambda <**value**> Value of chosen wavelength, in nm.

–wc_file <**name**> Name of water cloud file. Default none. Must be specified.

The following different types of tables may be generated.

Simple wavelength ratios with `Gen_wc_tab` The simplest type of table is made of the global irradiance at a single wavelength. This is the type of table described by Stamnes et al. (1991). This type of table is typically used to analyse measurements of the global irradiance from spectroradiometers. It is generated by the following command (is line continuation character)

```
perl Gen_wc_tab.pl --slitfunction slitfncfile --lambda 380. \
                   --file table.dat --wc_file ../examples/WC.DAT
```

Here `slitfncfile` is the name of the slit function file. It is a two column file where the first column is the wavelength (nm, in relative units) and the second column holds the slit function. The slit function must be normalized to unity at the center wavelength.

The generated table `table.dat` is read by `read_Stamnes_tab` for a measured global irradiance, `-r 10.0`, and solar zenith angle, `-s 30.0`, corresponding to the modelled ratio in the table. The table must be corrected for the Earth–Sun distance for the day of the measurement. This is achieved by specifying `-d 170`, where `170` is the day number. The table is generated for day 1.

```
read_o3_tab -r 10.0 -s 30.0 -d 170 table.dat
```

Bandpassed wavelength ratios with Gen_wc_tab Instead of using a single wavelength it may be of advantage to use irradiances covering a certain wavelength range and weighted with a bandpass function. This approach may reduce problems due to changes in cloud cover and experimental uncertainties. This approach is also suitable to calculate cloud optical depth from multichannel, moderate bandwidth filter instruments (Dahlback, 1996). Such tables are generated by

```
perl Gen_wc_tab.pl --slitfunction slitfncfile  --lambda 380.0 \
                   --file table.dat --bandpass bp.dat
```

Here `bp.dat` is the bandpass function of the wavelength region. The bandpass file have two columns. The first column is the wavelength in nm and relative units to –lambda. If absolute units are specified as for filter instruments, use the –absolute option. The second column is the bandpass function.

The tables are read in the same way as the simple wavelength irradiance tables.

Chapter 6

Complete description of input options

6.1 Radiative transfer tool - `uvspec`

The `uvspec` input file consists of single line entries, each making up a complete input to the `uvspec` program. First on the line comes the parameter name, followed by one or more parameter values. The parameter name and the parameter values are separated by white space. Filenames are entered without any surrounding single or double quotes. Comments are introduced by a `#`. Blank lines are ignored. The order of the lines is not important, with one exception: if the same input option is used more than once, the second one will usually over-write the first one. Be aware that also options in another `included` input file will overwrite options specified before.

Since libRadtran version 1.8 input option names have changed. See section 3.1.4 on how to translate old style input files to new style input files.

The various input parameters are described in detail below.

aerosol_angstrom

Scale the aerosol optical depth using the Ångström formula:

$$\tau = \beta\lambda^{-\alpha} \tag{6.1}$$

where λ is in units of micrometer (Angström, 1929). Specify the Ångström alpha and beta coefficients by

```
aerosol_angstrom alpha beta
```

The optical thickness defined here is the integral from the user-defined `altitude` to TOA (top of atmosphere).

aerosol_default

Set up a default aerosol according to Shettle (1989). The default properties are a rural type aerosol in the boundary layer, background aerosol above 2km,

spring-summer conditions and a visibility of 50km. These settings may be modified with `aerosol_haze`, `aerosol_vulcan`, `aerosol_season`, and `aerosol_visibility`.

aerosol_file

Location of file defining aerosol optical properties.

```
aerosol_file type file
```

`type` defines the file type, which can be one of the following:

gg

Location of aerosol asymmetry parameter file.

The file must have two columns. Column 1 is the altitude in km. Column 2 is the asymmetry parameter of each layer. The asymmetry parameter defined with this option is constant with wavelength. If you require spectral dependence please use `aerosol_file explicit`. Comments start with `#`. Empty lines are ignored.

ssa

Location of aerosol single scattering albedo file.

The file must have two columns. Column 1 is the altitude in km. The altitude grid must be exactly equal to the altitude grid specified in the file `atmosphere_file`. Column 2 is the single scattering albedo of each layer. The single scattering albedo defined with this option is constant with wavelength. If you require spectral dependence please use `aerosol_file explicit`. Comments start with `#`. Empty lines are ignored.

tau

Location of aerosol optical depth file.

The file must have two columns. Column 1 is the altitude in km. The altitude grid must be exactly equal to the altitude grid specified in the file `atmosphere_file`. Column 2 is the aerosol optical depth of each layer. To allow wavelength-dependent aerosol optical thickness please use either `aerosol_angstrom` or `aerosol_file explicit`. Comments start with `#`. Empty lines are ignored.

moments

Set the aerosol phase function moments to the values specified in the aerosol moments file.

The file contains one column with arbitrary number of Legendre terms of the phase function. The phase function $p(\mu)$ is

$$p(\mu) = \sum_{m=0}^{\infty} (2m+1) \cdot k_m \cdot P_m(\mu) \tag{6.2}$$

where k_m is the m'th moment and $P_m(\mu)$ is the m'th Legendre polynomial. If not specified, a Henyey-Greenstein phase function is assumed where the asymmetry parameter g is either a default value depending on

the aerosol type or it may be specified using `aerosol_modify set gg`. The phase function will be the same for all altitudes and wavelengths. See `aerosol_file explicit` if more flexibility is wanted. May only be used together with the `disort` or `fdisort2` solver in combination with the option `disort_intcor moments`.

explicit

A way to specify aerosol optical depth, single scattering albedo, and phase function moments for each layer.

The file must have two columns where column 1 is the altitude in km. The second column is a the name of a file which defines the optical properties of the layer starting at the given altitude. The files specified in the second column must have the following format:

Column 1: The wavelength in nm. These wavelengths may be different from those in `source solar file`. Optical properties are interpolated to the requested wavelengths.

Column 2: The extinction coefficient of the layer in units km-1.

Column 3: The aerosol single scattering albedo of the layer.

Column 4-(nmom+4): The moments of the aerosol phase function.

For some simple examples see the files `examples/AERO_*.LAYER`. Note that if using the `rte_solver disort` it makes good sense to make the number of moments larger than `number_of_streams`. For `rte_solver fdisort1` the number of moments included in the calculations will be `number_of_streams`+1. Higher order moments will be ignored for these solvers. Please note that the uppermost line of the `aerosol_file explicit` denotes simply the top altitude of the uppermost layer. The optical properties of this line are consequently ignored. There are two options for this line: either an optical property file with zero optical thickness is specified or "NULL" us used.

aerosol_haze

Specify the aerosol type in the lower 2 km of the atmosphere as

```
aerosol_haze type
```

where `type` is an integer identifying the following aerosol types:

1 Rural type aerosols.

4 Maritime type aerosols.

5 Urban type aerosols.

6 Tropospheric type aerosols.

For a description of the different aerosol types see Shettle (1989).

aerosol_king_byrne

Scale the aerosol optical depth using the King Byrne formula (King and Byrne, 1976):

$$\tau(\lambda) = e^{\alpha_0} \cdot \lambda^{\alpha_1} \cdot \lambda^{\alpha_2 ln(\lambda)} \tag{6.3}$$

where λ is in units of micrometer (Angström, 1929). Specify the King Byrne $alpha_0$, $alpha_1$ and $alpha_2$ coefficients by

```
aerosol_king_byrne alpha_0 alpha_1 alpha_2
```

The optical thickness defined here is the integral from the user-defined `altitude` to TOA (top of atmosphere).

aerosol_modify
Modify aerosol optical properties.

```
aerosol_modify variable scale/set value
```

This option is identical to `wc_modify`. Please refer to `wc_modify` for a detailed description of `variable`.

aerosol_profile_modtran
Squeeze aerosol profile up to 6 km when altitude is non-zero as in MODTRAN. Per default the aerosol profile is shifted upwards and remains unchanged.

aerosol_season
Specify season to get appropriate aerosol profile.

```
aerosol_season season
```

where `season` is either `1` or `2`:

1 Spring-summer profile.

2 Fall-winter profile.

aerosol_set_tau_at_wvl
Set the aerosol optical thickness at wavelength lambda (nm). Other wavelengths are scaled accordingly. Note that this option requires for technical reasons that the wavelength interval defined by `wavelength` does contain `lambda`. The optical thickness defined here is the integral from the user-definded `altitude` to TOA (top of atmosphere).

```
aerosol_set_tau_at_wvl lambda tau
```

aerosol_species_file
Specify mass density profiles of a mixture of aerosol types.

```
aerosol_species_file profile [aero_1 aero_2 ...  aero_n]
```

where `aero_1` to `aero_n` are the aerosol species to be included. For each of these

species, the optical properties are read from the `aerosol_species_library`. If `aerosol_species_library` is not definded, the default library OPAC which can be obtained from the libRadtran website is used. The profile file needs to include vertical profiles for each of these species. This file can be either in *netCDF*-format (automatically recognized filename extension `.nc` or `.cdf`) or in ASCII format. The format of the ASCII file is:

```
 z1 dens(aero_1, z1) dens(aero_2, z1) ...  dens(aero_n, z1)
z2 dens(aero_1, z2) dens(aero_2, z2) ...
.  .  .
.  .  .
```

where `z` is the height in km, and `dens` are the aerosol mass densities in g/m3. Please make sure to include one column for each of the species `aero_1` to `aero_n` listed after `aerosol_species_file`. For netCDF input it is also possible to specify the unit 'kg kg^{-1}'; the data are then automatically converted to g/m^3.

Some default aerosol mixtures are provided, corresponding to the definitions in Hess et al. (1998). They can simply be invoked by

```
aerosol_species_file mixture_name
```

where `mixture_name` can be one of the following:

```
continental_clean
continental_average
continental_polluted
urban
maritime_clean
maritime_polluted
maritime_tropical
desert
antarctic
```

A variation of the desert mixture containing nonspherical particles is

```
desert_spheroids
```

aerosol_species_library

With this option the *directory* is specified where the optical property files for all aerosols species used in the `aerosol_species_file` are expected: For each species defined in `aerosol_species_file`, *netCDF*-file *species_name*`.nc`, (e.g. `INSO.nc`), which contains the optical properties of the aerosol species, has to be provided. The netcdf format is the one produced by the *libRadtran* `mie` tool.

The default library is OPAC (Hess et al., 1998), which is provided on the libRadtran webpage (Hess et al., 1998):

```
aerosol_species_library OPAC
```

OPAC contains following aerosol species:

```
INSO insoluble
WASO water_soluble
SOOT soot
SSAM sea_salt_accumulation_mode
SSCM sea_salt_coarse_mode
MINM mineral_nucleation_mode
MIAM mineral_accumulation_mode
MICM mineral_coarse_mode
MITR mineral_transported
SUSO sulfate_droplets
```

Variations of the mineral aerosol species containing nonspherical particles are:

```
MINM_SPHEROIDS mineral_nucleation_mode
MIAM_SPHEROIDS mineral_accumulation_mode
MICM_SPHEROIDS mineral_coarse_mode
```

The nonspherical mineral components are described by Koepke et al. (2015).

aerosol_visibility

Horizontal visibility in km. Affects the profile according to Shettle (1989) and the optical thickness.

```
aerosol_visibility value
```

aerosol_vulcan

Aerosol situation above 2 km as defined in Shettle (1989).

```
aerosol_vulcan value
```

where `value` is an integer choosing between the following models

1 Background aerosols.

2 Moderate volcanic aerosols.

3 High volcanic aerosols.

4 Extreme volcanic aerosols.

albedo

The Lambertian surface albedo

```
albedo value
```

where `value` is a number between 0.0 and 1.0, constant for all wavelengths. For wavelength dependent surface albedo use `albedo_file`. The default albedo is 0.0.

albedo_file

Location of surface albedo file for wavelength dependent surface albedo.

```
albedo_file file
```

The file must have two columns. Column 1 is the wavelength in nm, and column 2 the corresponding Lambertian surface albedo. An arbitrary wavelength grid may be chosen as the albedo will be interpolated linearely to the wavelength grid used for the radiation calculation. Comments start with #. Empty lines are ignored. A large collection of spectral albedos are available e.g. at http://speclib.jpl.nasa.gov/ (Baldridge et al., 2009).

albedo_library

Albedo libraries are a collection of spectral albedos of different surface types. This option must be used either with `bdrf_rpv_type` or `surface_type_map`, in order to select the specific surface type. There are two possibilities for libraries: the built-in IGBP library or a user defined albedo library.

The built-in library of the International Geosphere Biosphere Programme is selected with

```
albedo_library IGBP
```

The IGBP library contains 20 surface types which are set by `brdf_rpv_type`:

```
 1 evergreen_needle_forest
2 evergreen_broad_forest
3 deciduous_needle_forest
4 deciduous_broad_forest
5 mixed_forest
6 closed_shrub
7 open_shrubs
8 woody_savanna
9 savanna
10 grassland
11 wetland
12 cropland
13 urban
14 crop_mosaic
15 antarctic_snow
16 desert
17 ocean_water
18 tundra
19 fresh_snow
20 sea_ice
```

Surface types 1 - 17 are defined by the International Geosphere Biosphere Programme (IGBP); additionally there are tundra, fresh_snow, and sea_ice surface types. The spectral albedo of the ground is determined as a function of solar zenith angle, precitable water, and clouds. The spectral resolution equals the grid of the

correlated-k Fu/Liou parameterisation. This library originates from the NASA CERES/SARB Surface Properties Project, see Belward and Loveland (1996).

For creating your own albedo library use `albedo_library path`, where `path` is the path of the directory where the albedo data is stored. The files are expected to have the names `albedo_01.dat, albedo_02.dat, ...` If `brdf_rpv_type 1` is specified the albedo from `albedo_01.dat` will be used, and so on. Each file is required to have two columns: Column 1 is the wavelength in nm, and column 2 the corresponding Lambertian surface albedo. The wavelength grid may be freely set. The albedo will be interpolated linearely to the wavelength grid used for the radiation calculation. Comments start with `#`. Empty lines are ignored. This option is similar to `albedo_file`, except that it offers an easy way to use the option `surface_type_map` in combinition with albedo files.

altitude

Set the bottom level in the model atmosphere provided in `atmosphere_file` to be at the given altitude above sea level (km).

```
altitude 0.73 # Altitude of IFU, Garmisch-Partenkirchen
```

The profiles of pressure, temperature, molecular absorbers, ice and water clouds are cut at the specified altitude. The aerosol profile is not affected by `altitude` but starts right from the model surface. This is a convenient way for the user to calculate the radiation at other altitudes than sealevel. Note that `altitude` is very different from `zout` where the radiation is calculated at an altitude of zout above the surface. E.g. to calculate the radiation field 1 km above the surface at a location at 0.73 km above sealevel, one would specify '`altitude` 0.73' and '`zout` 1.0'. If an altitude is specified which is below the lowest level in the `atmosphere_file`, the atmospheric profiles are extrapolated assuming a constant gradient for temperature and mixing ratios. A second optional argument may be given to `altitude` as e.g.

```
altitude 0.73 0.5
```

Here the bottom level will be at 0.73 km and the vertical resolution of the model atmosphere will be redistributed to have a spacing between levels specified by the second number, here 0.5 km, starting however from 0km. (Levels 0.73, 1., 1.5 ... will be added to the original atmosphere grid and optical properties are devided into the new layers. In order to use interpolated properties use `zout_interpolate`. See verbose output for details.) Be aware that specifying a fine vertical spacing will produce many layers thus increasing the computing time. Also the radiative transfer equation solvers implemented in Fortran 77 might need to have some array sizes increased (see `src_f/DISORT.MXD`).

atm_z_grid

With this option the vertical resolution of the `atmosphere_file` data is changed to the levels (in km above sea surface) given as argument. This might be useful in oder to reduce the number of levels (save computational time) or in order to easily adjust the atmosphere profile to the resolution of a Monte Carlo cloud file `wc_file`

3D or ic_file 3D.

```
atm_z_grid 0 2 4 6 8 10 20 30 ...
```

atmosphere_file

Location of the atmospheric data file.

```
atmosphere_file file
```

The file must have at least three columns containing the altitude, pressure, and temperature. Missing profiles are filled with 0 (e.g., if you did not specify the ozone profile, there will be no ozone absorption!), with exception of the air density which is calculated from pressure and temperature. Other trace gases may be set by mol_file. The columns are interpreted as follows:

1 Altitude above sea level in km

2 Pressure in hPa

3 Temperature in K

4 air density in cm^{-3}

5 Ozone density in cm^{-3}

6 Oxygen density in cm^{-3}

7 Water vapour density in cm^{-3}

8 CO2 density in cm^{-3}

9 NO2 density in cm^{-3}

The atmosphere is specified top-down, that is, the top level is the first line in the file, the bottom (surface) level the last line. All properties refer to model *level* z, not to model *layer*. It is important that the correct units are used, otherwise unpredictable results are guaranteed. Comments start with #. Empty lines are ignored. Please note that there is some redundancy: For air as an ideal gas the density ρ, can be calculated from pressure and temperature, $\rho = p/kT$. uvspec will check if this relation is fulfilled and will stop if it is not. *libRadtran* provides the six standard atmospheres by Anderson et al. (1986):

afglt Tropical (tropics)

afglms Midlatitude Summer (midlatitude_summer)

afglmw Midlatitude Winter (midlatitude_winter)

afglss Subarctic Summer (subarctic_summer)

afglsw Subarctic Winter (subarctic_winter)

afglus U.S. Standard (US-standard)

which may be chosen by for example

```
atmosphere_file tropics
```

or by specifying the full file name. These atmosphere files are found in `data/atmmod`. If no `atmosphere_file` is defined, *uvspec* will automatically select one. If the information `time`, `latitude` and `longitude` are provided in the input file *uvspec* will choose from the first 5 files, otherwise it takes the U.S. Standard atmosphere.

bpdf_litvinov

Land BPDF using the model of Litvinov et al. (2012) with a small modifications to correct for coherent backscattering. Here `albedo` is the black sky albedo, `rms_slope` the root mean square of slopes at the first scale, `fresnel` the portion of surface elements that can provide Fresnel scattering, and `shadowing` the shadow parameter. Optionally the real part of the refractive index `refr_index` along with its imaginary part `refr_index_i` can be provided. By default it is set to $1.5 + 0i$ which is a common assumption in surface models. Also unless explicitly specified the root mean square at the second scale `rms_slope2` is assumed to be 0.9. Please read Litvinov et al. (2012) for equations and detailed descrption of the input parameters. The code has been adapted from the GRASP software (Dubovik et al., 2014).

```
bpdf_litvinov albedo rms_slope fresnel shadowing refr_index
refr_index_i rms_slope2
```

bpdf_maignan

Land BPDF using Maignan and Breon's model. The model is based on Maignan et al. (2009) and was adapted to be used in a reflection matrix and utilizes an RPV model for its first matrix element. So be sure to also provide `brdf_rpv` or `brdf_rpv_file`. The parameter `c_maign` describes the single empirical parameter of this model. Optionally `arvi` is the ARVI or NDVI. If not specified a value of zero is assumed. As with `bpdf_litvinov` the refractive index can also be provided and defaults to $1.5 + 0i$. The code has been adapted from the GRASP software (Dubovik et al., 2014).

```
bpdf_maignan c_maign arvi refr_index refr_index_i
```

bpdf_tsang_u10

Wind speed for ocean BPDF (in m/s) at present only available with `rte_solver mystic`.

```
bpdf_tsang_u10 value
```

The BPDF model has been developed by Tsang et al. (1985). The wind

speed is the most important parameter affecting the ocean reflectance matrix. The BPDF model also takes into account shadowing by surface waves. The model has been implemented in a FORTRAN routine by Mishchenko (http://www.giss.nasa.gov/staff/mmishchenko/brf/) which has been included into *libRadtran*.

brdf_ambrals

AMBRALS (Ross-Li) BRDF, a three-parameter BRDF fit for vegetated and non-vegetated surfaces (Roujean et al., 1992; Wanner et al., 1997; Lucht et al., 2000; Schaaf et al., 2002), based on the RossThickLiSparseReciprocal model. The implementation is according to Lucht et al. (2000).

```
brdf_ambrals variable value
```

`variable` can be one of the following:

iso f_iso, Eq. (37) Lucht et al. (2000).

vol f_vol, Eq. (37) Lucht et al. (2000).

geo f_geo, Eq. (37) Lucht et al. (2000).

The hot spot correction factor introduced by Maignan et al. (2004) can be turned on by the option `brdf_ambrals_hotspot`. May be combined with `mystic`, `disort`, and `fdisort2`.

brdf_ambrals_file

4 column file, containing the AMBRALS (Ross-Li) BDRF parameterization, see `brdf_ambrals`.

```
brdf_ambrals_file file
```

This option is only supported with solvers: `disort` and `rte_solver mystic`. The columns of the input file are wavelength [nm], iso, vol, and geo. The parameters are interpolated linearly to the internal wavelength grid. To make sure that the results are reasonable, specify the Ambrals data on a wavelength grid similar or equal to that used internally for the radiative transfer calculation!

brdf_ambrals_hotspot

Turn on hot spot correction factor by Maignan et al. (2004) when using the AMBRALS (Ross-Li) BRDF.

brdf_cam

Set Cox and Munk (1954a,b) ocean BRDF properties.

```
brdf_cam variable value
```

`variable` can be one of the following:

pcl

Pigment concentration for Cox and Munk (1954a,b) ocean BRDF (in mg/m^{-3}). The default value is 0.01 mg/m^{-3}.

sal

Salinity for Cox and Munk (1954a,b) ocean BRDF (in "per mille", 0.1%; this unit is equivalent to the other common units for salinity, ppt - parts per thousand, psu - practical salinity unit). The default value is 34.3.

u10

Wind speed for Cox and Munk (1954a,b) ocean BRDF (in m/s). The wind speed is the most important parameter affecting ocean BRDF. The minimum allowed wind speed is 1 m/s because otherwise the strong specular reflection causes numerical problems. If a lower value is specified, the wind speed is automatically set to 1m/s.

uphi

Wind direction for Cox and Munk (1954a,b) ocean BRDF. Default value is 0 degrees, which is wind from the South. 90 degrees corresponds to wind from the West, etc. (Honestly, this was never truly validated. It could possibly be that 0 is wind from the North, 90 is wind from the East, etc.) The option is only implemented for the `mystic` solver.

At present only available with `rte_solver disort`, `rte_solver mystic` and `rte_solver fdisort2`. The number of streams (`number_of_streams`) is automatically increased to 16 if `cox_and_munk` BRDF is switched on, to avoid numerical problems. To switch on Cox and Munk BRDF, specify any of the `brdf_cam` options and define at least `brdf_cam u10`. Works also with polarization.

brdf_cam_solar_wind

Use old definition of wind direction for Monte Carlo simulations. If this switch is set, the wind azimuth is identical to the incoming photon azimuth. Else, the wind azimuth is set by `brdf_cam uphi` or is 0 by default.

brdf_hapke

Wavelength-independent Hapke BRDF values. Hapke is a parameterization of extraterrestial solid bodies such as the moon, asteroids or the inner planets by Hapke (1993).

```
brdf_hapke variable value
```

`variable` can be one of the following:

w Single scattering albedo of surface.

B0 Hot spot factor.

h Surface roughness parameter.

brdf_hapke_file

4 column file, containing the Hapke BDRF parameterization, see `brdf_hapke`.

```
brdf_hapke_file file
```

This option is only supported with solvers: `disort` and `rte_solver mystic`. The columns of the input file are wavelength [nm], w, B0, and h. The parameters are interpolated linearly to the internal wavelength grid. To make sure that the results are reasonable, specify the Hapke data on a wavelength grid similar or equal to that used internally for the radiative transfer calculation!

brdf_rpv

Wavelength independent RPV values, see `brdf_rpv_file`.

```
brdf_rpv variable value
```

`variable` can be one of the following:

k Overwrite the wavelength-dependent k value defined in `brdf_rpv_file`.

rho0 Overwrite the wavelength-dependent rpv0 value defined in `brdf_rpv_file`.

theta Overwrites the wavelength-dependent theta value defined in `brdf_rpv_file`.

sigma Constant RPV sigma, to be used for snow (Degünther and Meerkötter, 2000).

t1 Constant RPV t1, to be used for snow (Degünther and Meerkötter, 2000).

t2 Constant RPV t2, to be used for snow (Degünther and Meerkötter, 2000).

scale Apply a constant scaling factor for the RPV BRDF. Required e.g. if the the albedo should be set to a certain value. This factor is only used by `rte_solver disort`, `rte_solver fdisort2` and `rte_solver mystic`.

brdf_rpv_file

4 to 7 column file, containing the Rahman, Pinty, and Verstraete (RPV) BDRF parameterization (Rahman et al., 1993a) and the snow extension by (Degünther and Meerkötter, 2000).

```
brdf_rpv_file file
```

Bidirectional reflectance distribution functions for a variety of surfaces are given in the paper. This option is only supported with solvers: `disort`, `fdisort2` and `rte_solver mystic`. The columns of the input file are wavelength [nm], rho0, k, and theta. The parameters are interpolated linearly to the internal wavelength grid. To make sure that the results are reasonable, specify the RPV data on a wavelength grid similar or equal to that used internally for the radiative transfer calculation! Optionally, a fifth column with a constant scaling factor may be defined. If it has seven columns, the fifth to seventh are sigma, t1, t2, and if it has eight, the eighth is scale again.

brdf_rpv_library

The rpv libraries are collections of spectral BRDFs of different surface types, This

option must be used either with `brdf_rpv_type` or `surface_type_map`, in order to select the specific surface type.

For using a `brdf_rpv_library` write

```
brdf_rpv_library library_path
```

where `library_path` is the path of the directory, where the BRDF data is stored. The files are expected to have the names `IGBP.01.rpv, IGBP.02.rpv, ...` If `brdf_rpv_type 1` is specified the BRDF from `IGBP.01.rpv` will be used, and so on. Each file must have the structure like an `brdf_rpv_file`. (This option is quite the same as `brdf_rpv_file`, except that it offers you an easy way to use the option `surface_type_map` in combinition with your `brdf_rpv_files`.)

```
brdf_rpv_library IGBP
```

The built-in library contains the first 17 surface types see `albedo_library`. The data is given for the wavelengths 443nm, 565nm, 670nm, and 865nm. Stay near this wavelength in order to get reasonable results. In future this the rpv-library will be NDVI dependent, but until now the most common NDVI class is selected automatically.

brdf_rpv_type

With this option the (RPV) BRDF surface type is selected. This option can be used with `albedo_library` in order to select a spectral albedo or with `brdf_rpv_library` in order to select a BRDF function.

```
brdf_rpv_type surface_type_number
```

where `surface_type_number` is an integer starting from 0, where 0 refers to a black surface and the following numbers to the entries in the specified `library`.

ck_lowtran_absorption

Switch off absorption by individual minor trace gases which are currently only included when `mol_abs_param lowtran` is chosen. The syntax is

```
ck_lowtran_absorption species on/off
```

where species may be one of O4, N2, CO, SO2, NH3, NO, HNO3. By default all are switched on.

This option may also be used to turn on/off absorption by O4 in spectral resolution. It is on by default.

cloud_fraction_file

File containing a cloud fraction profile.

```
cloud_fraction_file file
```

Two columns are expected: altitude [km] and cloud fraction, including ice and water clouds. If `cloud_fraction_file` is defined, effective cloud properties are calculated assuming either random overlap or maximum random overlap of the cloud layers (see also `cloud_overlap`). An example is provided in `examples/CF.DAT`.

cloud_overlap
Cloud overlap assumption.

```
cloud_overlap type
```

Following types are implemented:

rand Random overlap of cloud layers

maxrand Maximum random overlap scheme

max Maximum overlap scheme

off Turn off cloud overlap for ECMWF clouds

Per default the `cloud_overlap` scheme is switched off.

cloudcover
Set the fraction of the horizontal sky area which is covered by clouds.

```
cloudcover typename value
```

`typename` describes the name of the cloud type, which can be "wc" and "ic":

ic Cloud cover of ice cloud, where the cloud properties are taken from `ic_file`.

wc Cloud cover of water cloud, where the cloud properties are taken from `wc_file`.

When a cloud cover is specified, the result will be calculated by the independent pixel approximation (IPA), that is, as weighted average of cloudless sky and overcast sky. Please note that, if both `cloudcover ic` and `cloudcover wc` are set, both must be equal.

This option is ignored, if the option `cloud_fraction_file` is used.

crs_file
May be used to specify cross sections of O3, O2, H2O, CO2, NO2, BRO, OCLO, HCHO, O4, SO2, CH4, N2O, CO, or N2 to be used instead of those supplied with *libRadtran*. No temperature dependence may be specified. Use as follows:

```
crs_file NO2 ../examples/no2_crs.dat
```

The species, e.g. `NO2`, must be specified to identify the species for which the cross section applies. The cross section file has two columns:

1 wavelength (nm)

2 cross section (cm^2)

crs_model

Choose between various cross sections.

```
crs_model species crs
```

Following `species` are included:

rayleigh

Specify the Rayleigh cross section. Choose between the following Rayleigh scattering cross sections (`crs`):

Bodhaine Bodhaine et al. (1999) Rayleigh scattering cross section using their Eqs. 22-23.

Bodhaine29 Bodhaine et al. (1999) Rayleigh scattering cross section using their Eq. 29.

Nicolet Nicolet (1984) Rayleigh scattering cross section.

Penndorf Penndorf (1957) Rayleigh scattering cross section.

Bodhaine et al. (1999) is default.

o3

Choose ozone cross section. `crs` can be one of the following:

Bass_and_Paur Bass and Paur (1985) ozone cross section.

Molina Molina and Molina (1986) ozone cross section.

Daumont Ozone cross section by Daumont et al. (1992), Malicet et al. (1995).

Bogumil Ozone cross section from Bogumil et al. (2003).

Serdyuchenko Ozone cross section from Serdyuchenko.

Molina and Molina (1986) is default.

no2

Choose between the various NO2 cross sections. `crs` is one of:

Burrows Burrows et al. (1998) NO2 cross section.

Bogumil NO2 cross section from Bogumil et al. (2003).

Vandaele NO2 cross section from Vandaele et al.

Burrows et al. (1998) is default.

o4

Choose between the various O4 cross sections. `crs` is one of:

Greenblatt O4 cross section by Greenblatt et al. (1990).

Thalman O4 cross section by Thalman and Volkamer (2013).

data_files_path

The path to the directory where all `uvspec` internal data files live, e.g. the files that are in the subdirectories of the `data` directory that comes with the `uvspec` distribution.

```
data_files_path path
```

The default for `path` is `../data/`.

day_of_year

Integer, to correct the calculated radiation quantities for the Sun-Earth distance for the specified Julian day (1-365).

```
day_of_year value
```

If not specified, the Earth-Sun distance is 1 AU (i.e. equinox distance), that is, no correction is applied to the extraterrestrial irradiance `source solar file`. Alternatively `time` may be used for that purpose.

deltam

Turn delta-M scaling on/off. Set to either `on` or `off`. Note that for the `rte_solver disort` and `rte_solver fdisort2` delta-M scaling is hardcoded to be always on.

disort_intcor

Intensity correction method for `rte_solver disort` or `rte_solver fdisort2`. Valid options are `phase`, i.e. the phase function is used for the Nakajima intensity correction, and `moments`, i.e. the Legendre moments are used for the correction. Optionally, the option `off` turns off the intensity correction. Default is `phase`.

earth_radius

Specify the earth radius in km.

```
earth_radius value
```

This is needed by all solvers in spherical geometry, e.g. `mystic` in combination with option `mc_spherical`. The default value is 6370 km.

filter_function_file

If specified, the calculated spectrum is multiplied with a filter function defined in file.

```
filter_function_file file [normalize]
```

The file must contain two columns. Column 1 is the wavelength, in nm. Column 2 is the corresponding filter function value. Comments start with `#`. Empty lines are ignored. In combination with `output_process sum` or `output_process integrate` this option is useful e.g. to calculate weighted irradiances or actinic fluxes or to simulate broadband or satellite observations.

If the optional second argument `normalize` is specified, the integral of the filter function over wavelength is normalized such that `output_process integrate` gives radiative properties per wavelength, averaged over the filter function.

fluorescence

Specifies the magnitude of a bottom surface isotropic fluorescence source.

```
fluorescence value
```

where value is a number greater or equal to 0.0, constant for all wavelengths. Must be used together with source solar file. The units of the fluorescence should obviously be the same as for the solar source in source solar file. For wavelength dependent fluorescence use fluorescence_file. The default fluorescence is 0.0. Currently only works with the disort solver.

fluorescence_file

Location of fluorescence file for wavelength dependent fluorescence emission from the bottom surface.

```
fluorescence_file file
```

The file must have two columns. Column 1 is the wavelength in nm, and column 2 the corresponding fluorescence. An arbitrary wavelength grid may be chosen as the fluorescence will be interpolated linearely to the wavelength grid used for the radiation calculation. Comments start with #. Empty lines are ignored. Currently only works with the disort solver. Furthermore. if raman is not set, wavelength_grid_file must be specified with the same resolution as the source solar file, and the first value must be the value specified by wavelength. The units of the fluorescence should obviously be the same as for the source solar file.

heating_rate

Calculation of heating rates. Output is only provided at altitudes specified by zout. To get heating rate profiles a number of altitudes must thus be specified by zout. Heating rates is the change of temperature with time in units of K/day. For spectral calculations the default output is a matrix:

```
0.0          zout1           zout2 ...
lambda1      heating\_rates   ...
lambda2        .
   .           .
   .           .
```

For integrated calculations (output_process sum or output_process integrate) the default output is in two columns with column 1 being the altitude and column 2 the heating rates. The output of heating_rate can also be specified with the output_user option. Note that heating rates are only well-behaved up to altitudes for which the respective correlated-k options are valid. E.g. about 60 km for fu and about 80 km for kato, kato2, kato2.96, and lowtran. Attention: For spectral calculations, the extraterrestrial spectrum is assumed to be in mW/(m2 nm).

Three different methods are implemented to calculate the heating rate, which can be selected with an optional keyword:

```
heating_rate [method]
```

where method may be either layer_fd (heating rates are derived from forward differences of the flux over one layer, that's the default), layer_cd (heating rates are derived from centered differences of the flux), or local (heating rates are derived from the actinic flux). Attention: heating_rate local introduces new levels into the profile which slightly affects the model output. With layer_fd, the output is representative for the *layer* between the z-level in the output file to the *output level* above.

ic_file

Location of file defining ice cloud properties.

```
ic_file type file
```

type defines the file type, which is identical to wc_file type. See wc_file for choices of type and a description on the file structures.

ic_fu

```
ic_fu reff_def on/off
```

Specify wich definition of the effective radius is used.

If on the parameterization uses the original definition of the effective radius as specified in Fu (1996); Fu et al. (1998).

Default is off. The same definition of the effective radius is used as the Key et al. (2002), Yang et al. (2000) and Baum et al. (2005a,b) parameterizations; see discussion of ic_properties.

```
ic_fu deltascaling on/off
```

Specify if the Fu (1996) optical properties are delta-scaled or not.

If on delta-scaling is switched on.

If off delta-scaling is switched off. The default is without delta-scaling. Please note that this was changed on July 22, 2008: Before, delta-scaling was switched on by default which might have caused some confusion, because irradiance calculations were not consistent with the other ice cloud parameterizations implemented in uvspec. Using the Fu (1996) parameterization in combination with one of ic_modify you now get consistent results with all other ice cloud parameterizations.

ic_habit

Ice crystal habit for the Yang et al. (2000), Key et al. (2002) and hey parameterizations, see also ic_properties key/yang/hey.

```
ic_habit type
```

For Key/Yang `type` may be one of `solid-column`, `hollow-column`, `rough-aggregate`, `rosette-4`, `rosette-6`, `plate`, `droxtal`, `dendrite` and `spheroid`. Please note that this parameterization is only valid for a restricted size range, depending on the habit (see table 1 in Key et al. (2002). Also, some of the habits are only available for wavelengths below 5 micrometer (`rosette-4`) while others are only available for wavelengths larger than 3 micrometer (`droxtal`, `spheroid`).

For `hey` the following habits can be chosen: `solid-column`, `hollow-column`, `rough-aggregate`, `rosette-6`, `plate`, `droxtal`, and the general habit mixture `ghm` which follows the "recipe" by Baum et al. (2005a). All habits and the habit mixture are available for effective radii from 5 to 90 micrometers in the wavelength region from 0.2 to 5 micrometers.

The parameterization `baum_v36` includes the general habit mixture `ghm` and the habits `solid-column` and `aggregate`, all crystals modeled with severe roughness.

ic_habit_yang2013

Ice crystal habit for the Yang et al. (2013) parameterization, `ic_properties yang2013`.

```
ic_habit type roughness
```

The following habits are available: `column_8elements`, `droxtal`, `hollow_bullet_rosette`, `hollow_column`, `plate`, `plate_10elements`, `plate_5elements`, `solid_bullet_rosette`, and `solid_column`.

For each habit three degrees of roughness needs to be specified, options are `smooth`, `moderate` and `severe`.

ic_modify

Modify ice cloud optical properties.

```
ic_modify variable scale/set value
```

This option is identical to `wc_modify`. Please refer to `wc_modify` for a detailed description of `variable`.

If you use this option in combination with the ice cloud properties by Fu (1996), please make sure that you understand the explanation of `ic_fu`.

ic_properties

Defines how ice water content and effective particle radius are translated to optical properties.

```
ic_properties property [interpolate]
```

Possible choices for `property` are

fu

Parameterization by Fu (1996); Fu et al. (1998), see `ic_file`; this is the default setting. Note that this is a parameterization which has been created to calculate fluxes but not radiances. Note also that the optical properties in the solar range provided by Fu (1996) are delta-scaled properties (that is, the forward peak of the phase function is truncated and optical thickness, asymmetry parameter, and single scattering albedo are reduced accordingly), whereas `uvspec` uses non delta-scaled properties unless the option `ic_fu deltascaling on` is specified. By default the parameterization by Fu (1996) is treated consistently with all other ice cloud parameterizations. For wavelengths up to 4 micrometer Fu (1996) is used while for wavelengths larger than 4 micrometer Fu et al. (1998) is chosen. Please note that Fu (1996) is based on ray-tracing calculations while Fu et al. (1998) is a mixture of ray-tracing and Mie calculations (which is required for the infrared wavelengths where the geometrical assumption does not hold). Hence, both parameterizations are not fully consistent. Rather, differences of some % are to be expected in the wavelength region where both parameterizations overlap. Also, the wavelength dependence in the solar and infrared parts is treated differently: In the solar part (Fu, 1996) the optical properties are defined for wavelength bands - hence they are assumed constant within each band. In the infrared (Fu et al., 1998) they are defined at certain wavelengths and linearely interpolated in between. If you use this option, please see also the discussion of `ic_fu deltascaling` and `ic_fu reff_def`. The allowed range for the effective radius is from 9.315 - 65.120 micrometer.

echam4

Use the simple two-band parameterization of the ECHAM4 climate model, described in Roeckner et al. (1996); this is probably only meaningful if you want to compare your results with ECHAM4, the two bands are 0.2 - 0.68 micrometer and 0.68 - 4.0 micrometer. Within the two ECHAM4 bands, the optical properties are assumed constant.

key

Parameterization by Key et al. (2002). This parameterization can also be used to calculate radiances because it uses a double-Henyey-Greenstein phase function which better represents both forward and backward peaks. This parameterization covers the wavelength region from 0.2 to 5.0 micrometer and is available for the following `habit: solid-column`, `hollow-column`, `rough-aggregate`, `rosette-4`, `rosette-6`, and `plate`.

yang

Parameterization similar to Key et al. (2002) but based on more recent single scattering calculations. Below 3.4 micrometer it actually equals the Key et al. (2002) parameterization while from 3.4 - 100 micrometer new coefficients have been calculated with much higher wavelength resolution and better accuracy. Hence, `yang` should give a reasonably consistent approximation from 0.2 - 100 micrometer, suitable for spectrally resolved calculations of radiance and irradiance. The covered range for the effective radius depends on the `ic_habit`.

(In micrometer: `solid-column` [5.96, 84.22], `hollow-column` [4.97, 70.24], `rough-aggregate` [3.55, 108.10], `rosettes-4` [2.77, 45.30], `rosettes-6` [2.85, 46.01], `plate` [4.87, 48.18], `dendrites` [0.45, 1.88], `droxtal` [9.48, 293.32], `spheroid` [6.58, 203.39]).

baum

Use ice cloud parameterization from Baum et al. (2005a,b), `http://www.ssec.wisc.edu/~baum/Cirrus/IceCloudModels.html`. In combination with the radiative transfer solvers `disort`, `montecarlo`, and `fdisort2`, accurate phase functions are used.

baum_v36

Use cloud parameterization from Heymsfield et al. (2013); Yang et al. (2013); Baum et al. (2014) covering the spectral range from 0.2 to 100 μm and effective radii from 5 to 60 μm. The parameterization assumes severly roughened and randomly oriented ice particles and includes the full phase matrix. Three set of models are available, they can be selected using `ic_habit`: `ghm` is based on a general habit mixture involving 9 habits, `solid-column` assumes severely roughened solid columns, and `rough-aggregate` is based on severly roughened aggregates. The default is `solid-column`.

hey

Use pre-calculated ice cloud optical properties including full phase matrices. The parameterization is currently only available for the spectral region from 0.2 to 5 micrometers. The single scattering properties have been been generated by Hong Gang using the models by Yang et al. (2000). The parameterization is based on simple gamma distributions

$$n(r) = n_0 r^{\alpha} \exp\left(-\frac{(\alpha+3)r}{r_e}\right), \tag{6.4}$$

where n_0 is found by normalization and α is set to 1. In case of spherical particles the parameter r_e would be the effective radius. For aspherical particles, the parameter r_e is found iteratively so that the size distribution yields the required effective radius. The parameterization is availabe for the following habits: `solid-column`, `hollow-column`, `rough-aggregate`, `rosette-6`, `plate`, and `droxtal`. The default habit is `solid-column`. Furthermore a general habit mixture `ghm` similar to the one defined by Baum et al. (2005b) may be selected. For the HEY parameterization the ice crystals are assumed to be smooth, in contrast to the severely roughened particles assumed by `baum_v36`. The habit can be specified using the option `ic_habit`.

yang2013

Pre-calculated ice optical properties including full phase matrices for the spectral region from 0.2 to 99 μm. The parameterization uses single scattering data by Yang et al. (2013) and assumes gamma size distributions as the `hey` parameterization. It is available for 9 habits and 3 degrees of roughness, which can be selected using the option `ic_habit_yang2013`.

filename

Read optical properties from specified filename; file format is as produced by the `mie` tool of *libRadtran* (see `output_user netcdf`).

The default property is `fu`.

Please note also that, in contrast to spherical particles, there is no unique definition of effective size for non-spherical particles. In particular, the above parameterizations use different definitions which, however, differ only by a constant factor. Yang et al. (2000), Key et al. (2002), and Baum et al. (2005a,b) use the general definition

$$r_{\text{eff}} = \frac{3}{4}\frac{\int V(h)n(h)dh}{\int A(h)n(h)dh} \tag{6.5}$$

where h is the maximum dimension of an ice crystal, $n(h)$ is the number of particles with maximum dimension h in the size distribution, and V and A are the volume and mean projected area of the particles, respectively. The volume and area are based on the spherical diameter with equivalent volume and the spherical diameter with equivalent projected area as defined by Yang et al. (2000). On the other hand, Fu (1996); Fu et al. (1998) use hexagonal columns and use the following definition

$$r_{\text{eff}} = \frac{\int D^2 L n(L)dL}{2\int (DL + \frac{\sqrt{3}}{4}D^2)n(L)dL} \tag{6.6}$$

where D is the width of the ice crystal (that is, the maximum diameter of the hexagonal area) and L is the length. The integrand in the numerator is proportional to the volume while that in the denominator is proportional to the projected area. Evaluating these formulas one finds that, for the same hexagonal particle, the effective radius would be $3\sqrt{3}/4 = 1.299$ times larger following the Yang et al. (2000), Key et al. (2002) definition rather than the Fu (1996); Fu et al. (1998) definition. As an example, an effective radius of $20\mu m$ with `ic_properties fu` and `ic_fu reff_def on` and $1.299 \cdot 20\mu m = 26\mu m$ with `ic_properties yang` would give comparable results for hexagonal columns. To use the original definition of the effective radius by Fu (1996); Fu et al. (1998) use `ic_fu reff_def on`!

With the optional argument `interpolate` the ice cloud optical properties are interpolated over wavelength; useful for precalculated optical property files defined with `ic_properties`. Please note that this option may be extremely memory-consuming because for each internal wavelength a full set of Legendre moments of the phase function is stored (up to several thousands).

include

Include a file into the `uvspec` input.

```
include file
```

Works exactly like the C `#include` or the Fortran `INCLUDE` statements.

interpret_as_level

Interpret profile properties as level properties (this was the default behaviour before version 1.4).

```
interpret_as_level profile
```

profile can be either `wc`, `ic` or any profile type specified in `profile_file`.

If `interpret_as_level wc` is defined, a `wc_file` would be interpreted as follows:

```
#       z      LWC     R\_eff
#      (km)   (g/m^3)  (um)
        5.000     0       0
        4.000    0.2    12.0
        3.000    0.1    10.0
        2.000    0.1     8.0
```

The value 0.2 g/m^3 refers to altitude 4.0km, as e.g. in a radiosonde profile. The properties of each layer are calculated as average over the adjacent levels. E.g. the single scattering properties for the model layer between 3 and 4km are obtained by averaging over the two levels 3km and 4km. To allow easy definition of sharp cloud boundaries, clouds are only formed if both liquid water contents above and below the respective layer are larger than 0. Hence, in the above example, the layers between 2 and 3 as well as between 3 and 4km are cloudy while those between 1 and 2km and between 4 and 5km are not.

Note that since version 1.4 the default is to interpret profile properties as layer properties. For example wc properties are assumed to be constant over the layer. The layer reaches from the level, where the properties are defined in the `wc_file` to the level above that one. The following lines

```
#       z      LWC     R_eff
#      (km)   (g/m^3)  (um)
        4.000    0.0    0.0
        3.000    1.0   10.0
```

define a cloud in the layer between 3 and 4 km with sharp boundaries.

isotropic_source_toa

Specifies that isotropic illumination is used at top-boundary instead of beam source. Useful for those who want to calculate the reflectance for a homogeneous or inhomogeneous atmosphere. The intensity is still set by `source solar file`. Only works with `disort` and `twostr`.

latitude

This option can be used to specify the latitude of the location to simulate. (This option only has an effects, if `longitude` is specified, too.)

```
latitude N/S deg [min] [sec]
```

where N and S stands for the northern and southern hemisphere, respectively. deg min sec is the position in degrees, arc minutes, and arc seconds. deg might also be a float number. min and sec may be obmitted. The latitude information will be used for the following:

latitude in combination with longitude and time is used to calculate the solar zenith angle if no sza is specified.

latitude in combination with longitude and time is used to choose a suitable default atmosphere file, if no atmosphere_file is specified.

longitude

This option can be used to specify the longitude of the location to simulate. (This option only has an effects, if latitude is specified, too.)

```
longitude E/W deg [min] [sec]
```

where E and W stand for the eastern and western hemisphere, respectively. deg min sec is the position in degrees, arc minutes, and arc seconds. deg might also be a float number. min and sec may be obmitted. For possible usage of the longitude information, see latitude.

mc_azimuth_old

Use old MYSTIC azimuth convention (0 degree = looking from the direction of the sun; 180 degree = looking into the direction of the sun; that is, exactly opposite to the disort convention). The MYSTIC azimuth was changed March 1, 2004 - hence this option was introduced for compatibility reasons.

mc_backward

Backward tracing of photons. mc_backward takes either zero, two or four coordinates:

```
mc_backward [ix_start iy_start] [ix_end iy_end]
```

where ix_start, iy_start is the index of the sample pixel to be calculated or the pixel area from ix_start to ix_end and iy_start to iy_end. All x-indices must be in the range of 0 ... (Nx-1) and y-indices the range of 0 ... (Ny-1). If no coordinates are specified, all sample pixels will be calculated. mc_backward computes radiances and downward diffuse irradiances. If a different quantity is required, please use mc_backward_output.

mc_backward_increment

Backward tracing of photons. mc_backward_increment takes two integers:

```
mc_backward_increment ix_step iy_step
```

where ix_step, iy_step is the increment for the backward sampling. Pixels ix_start, ix_start + ix_step, ix_start + 2*ix_step (and similar for the y direction) are calculated. Defaults to 1.

mc_backward_output
Specify quantity to be calculated using backward Monte Carlo.

```
mc_backward_output output [unit]
```

So far the following `output` options have been implemented:

edir
direct horizontal irradiance

edn
diffuse downward irradiance (default)

eup
diffuse upward irradiance

exp
diffuse irradiance in positive x direction for grid box above specified altitude at the left (lower x) face; output is written to eup.

exn
diffuse irradiance in negative x direction for grid box above specified altitude at the left (lower x) face; output is written to edn.

eyp
diffuse irradiance in positive y direction for grid box above specified altitude at the front (lower y) face; output is written to eup.

eyn
diffuse irradiance in negative y direction for grid box above specified altitude at the front (lower y) face; output is written to edn.

act
actinic flux

abs
absorption

emis
emission

heat
heating rates, that is absorption + emission

For `abs`, `emis`, `heat` an optional argument `W_per_m2_and_dz` (default), `W_per_m3`, or `K_per_day` may be specified which converts the result e.g. to heating rates.

mc_backward_writeback
If set, the distribution of photons contributing to the result is written to a file with extension .bac which may be useful for some interpretations (it basically tells you where the photons come from whichn contribute to the result).

mc_basename
Filename for MYSTIC 3D output (default: mc).

```
mc_basename basename
```

mc_boxairmass

Calculate box-airmass-factors based on the pathlength distribution as described by Deutschmann et al. (2011). This option is currently only included for 1D atmospheres. The ouput is a two-column file (basename+.amf) including the altitude levels and the box-airmass-factors corresponding to the layer above the given altitude level. The altitude levels in the output file correspond to the once provided with `atmosphere_file` and the boxairmass factors are for the layers above the given altitude levels. The method works for trace gases which do not absorb a significant amount of radiation, i.e. which do not influence the pathlength distribution significantly.

mc_escape

Calculate MYSTIC radiances via escape probabilities; slows down the tracing but usually speeds up the computation considerably since it reduces noise. Switched on per default since it should basically be used always when calculating radiances. Only meaningful with `rte_solver montecarlo`. The syntax is

```
mc_escape on/off
```

mc_forward_output

Specify quantity to be calculated using forward Monte Carlo. Forward output is calculated for each grid box; may need a considerable amount of memory, depending on the 3D cloud grid. Only meaningful with `rte_solver mystic`. This option is only available for forward calculations. For backward please use `mc_backward_output`.

```
mc_forward_output quantity [unit]
```

`quantity` can be one of the following:

actinic

Calculate MYSTIC actinic flux by dividing the absorbed energy by the absorption coeffcient; this method is much better than the traditional photon counting which usually comprises spikes (because in the latter method each photon is weighted with $1/\cos(\theta)$ which may be a very large number); For backward please use `mc_backward_output act`.

heating

Calculate MYSTIC heating rates. This is identical to `absorption` for `source solar`. For `source thermal`, however, the emission of a photon in a grid box is counted as cooling. For backward please use `mc_backward_output heat`.

The optional argument `unit` may be one of `W_per_m2_and_dz` (default), `W_per_m3`, or `K_per_day`. `unit` may be specified to convert the result e.g. to heating rates.

mc_maxscatters
If set, photons are destroyed after n scatters. Please note that this is only for testing, debugging and process understanding! The result will certainly be wrong because photons are lost.

mc_minphotons
If set, this is the minimum value of photons to be used per simulation. The default value is `MIN_MCPHOTONS`, set in uvspec.h.

```
mc_maxscatters value
```

mc_minscatters
If set, local estimates are not performed before n scatters (e.g. if set to 1, single scattering is not taken into account). Please note that this is only for testing, debugging and process understanding! The result will certainly be wrong.

mc_nca
Approximate calculation of 3D thermal heating rates with the Neighbouring Column Approximation (Klinger and Mayer, 2016, 2019). For an example and a description how to define the 3D cloud input see `examples/UVSPEC_HEAT_NCA2019_*`.

mc_netcdf_surface_file

Use multiple models with spectral and spatial data in a single NetCDF file. Currently supported models are: Litvinov, Maignan, Lambertian surface and BPDF Tsang.

```
mc_netcdf_surface_file filename
```

mc_photons
Total number of photons to be traced by the Monte Carlo solver, MYSTIC.

```
mc_photons value
```

Only meaningful with `rte_solver montecarlo`.

mc_photons_file
Distribution of photons over wavelength bands; to be used with `mol_abs_param`.

```
mc_photons_file file
```

For an example see `data/correlated_k/kato2/x_solar.dat`. No

error checking! Do only use if you are absolutely sure what you are doing. Only meaningful with `rte_solver montecarlo`.

mc_polarisation

Switch on polarisation for `rte_solver montecarlo`. By default uses unpolarized sunlight (light starting with an initial Stokes Vector (1,0,0,0). Optionally you may provide one of the following numbers to specify one of the following initial Stokes Vectors:

- 0 : (1,0,0,0) (default)
- 1 : (1,1,0,0)
- 2 : (1,0,1,0)
- 3 : (1,0,0,1)
- -1 : (1,-1,0,0)
- -2 : (1,0,-1,0)
- -3 : (1,0,0,-1)
- 4 : Each photon's Stokes Vector is randomly determined fulfilling the condition $I^2 = Q^2 + U^2 + V^2$, use this e.g. if you need unpolarized radiation with `mc_coherent_backscatter` using `mc_lidar` or `mc_radar`. Averaging over a large number of these random Stokes Vectors leads again to unpolarized radiation (1,0,0,0).

Details about the implementation of polarisation are described in Emde et al. (2010).

mc_rad_alpha

Define opening angle for radiance calculations without local estimate. Ths oprion is useful for all-sky simulations. Default is 5 degrees.

mc_randomseed

Provide your own random seed (positive integer) for the random number generator.

```
mc_randomseed value
```

Usually a random seed is determined from current time plus process id. This option is useful to re-run a simulation for debugging.

mc_sensordirection

Define viewing direction of an irradiance sensor in Monte Carlo backward mode.

```
mc_sensordirection x-value y-value z-value
```

Has been introduced for irradiance calculations in topography and might not properly work with all options. For radiance use the usual `umu` and `phi`.

mc_spectral_is

Calculate a spectrum with high spectral resolution using an importance sampling method.

```
mc_spectral_is [wvl]
```

The spectral variation of Rayleigh scattering and molecular absorption is fully included as well the spectral variation of aerosol and cloud scattering and absorption coefficients. The spectral variation of the phase matrix is neglected, for all wavelengths the phase matrix of the calculation wavelength is assumed.

Use the optional argument `wvl` to specify calculation wavelength. If not set, the central wavelength of the selected spectral interval is used.

This method is very efficient for calculations with very high spectral resolution, e.g. simulations for trace gas retrievals, in particular when polarization is required. For more details refer to Emde et al. (2011).

mc_spherical

Spherical geometry in MYSTIC.

```
mc_spherical 1D
```

Works only in "1D" - `wc_file 3D` and `ic_file 3D` are not yet considered. If `mc_spherical` is selected `mc_backward` is switched on automatically. Viewing direction (`umu`, `phi`) and sun position (`sza`, `phi0`) are defined with respect to the sensor position specified by `zout`. For details about the implementation of spherical geometry please refer to Emde and Mayer (2007).

mc_surface_reflectalways

Usually, a photon is either absorbed or reflected at the surface, with a probability defined by the surface albedo. If `mc_surface_reflectalways` is specified, each photon is reflected and the albedo is considered by reducing the photon weight. In case of BRDF, `mc_surface_reflectalways` is switched on automatically because the other method is no longer implemented for non-Lambertian BRDFs, due to implementation and numerical problems. For small albedos, the computational time is increased if `mc_surface_reflectalways` is used; however, the accuracy of the upward radiance (reflected by the surface) is increased considerably. In case of clouds, however, computational time might be increased considerably without gaining accuracy.

mc_vroom

Variance Reduction Optimal Options Method (VROOM). Options are "on" and "off". Needs to be specified if you are calculating radiances and spiky phase functions are present in your atmosphere. If you are using VROOM, please cite: Buras and Mayer (2011).

mixing_ratio

Mixing ratio in ppm.

```
mixing_ratio species value
```

`species` can be one of the following:

O2 The mixing ratio of O2 in ppm. Scale the profile so that the mixing ratio at the user-defined `altitude` assumes the specified value.

H2O The mixing ratio of H2O in ppm. Scale the profile so that the mixing ratio at the user-define `altitude` assumes the specified value.

CO2 The mixing ratio of CO2 in ppm. Scale the profile so that the mixing ratio at the user-defined `altitude` assumes the specified value.

NO2 The mixing ratio of NO2 in ppm. Scale the profile so that the mixing ratio at the user-defined `altitude` assumes the specified value.

CH4 The mixing ratio of CH4 in ppm (default: 1.6 ppm).

N2O The mixing ratio of N2O in ppm (default: 0.28 ppm).

F11 The mixing ratio of F11 in ppm (default: 0.000268 ppm).

F12 The mixing ratio of F12 in ppm (default: 0.000503 ppm).

F22 The mixing ratio of F22 in ppm (default: 0.000105 ppm).

The `mixing_ratio` of F11, F12, and F22 and the default values for CH4 and N2O are ignored in case of `mol_abs_param reptran`.

mol_abs_param

To calculate integrated shortwave or longwave irradiance, or to simulate satellite instrument channels, use

```
mol_abs_param type
```

to choose between the following types of schemes:

reptran Representative wavelengths parameterization adapted for spectral bands. This parameterization is used by default if no `mol_abs_param` option is given in the *uvspec* input file. Different band widths may be selected by

```
mol_abs_param reptran [fine|medium|coarse|int]
```

(fine: 1cm^{-1}; medium: 5cm^{-1}; coarse: 15cm^{-1}, int: integrated; coarse is default). The data files for coarse resolution are included in the libRadtran package. The files required for fine and medium resolution can be downloaded from the libRadtran homepage. Absorption data is mainly based on HITRAN 2004. Absorption by H2O, CO2, O3, N2O, CO, CH4, O2, N2, and NO2 is considered, and absorption by all other gases is zero. By default volume mixing ratios of N2O, CO, CH4, and N2 (those are not in the `atmosphere_file`) from the US standard atmosphere are applied. Use `mol_file` or `mol_modify` to change the gas profiles. In case of radiative transfer problems with solar source, the extraterrestrial spectrum from Kurudz is applied by default. This parameterization is described in detail by Gasteiger et al. (2014). The absorption parameterization to be used for integrated irradiances and heating rates is described in de Mourgues et al. (2022) and Meier (2022).

reptran_channel Representative wavelengths parameterization for satellite channels. Usage

```
mol_abs_param reptran_channel channel_name
```

Channel-integrated quantities are obtained using `output_process per_band`. The file `data/correlated_k/reptran/channel_list.txt` provides a list of available channels; more information on the channels is provided in `data/filter/`. See Gasteiger et al. (2014) for details about the approach.

crs Switch off spectral parameterizations. Only molecular absorption cross sections from `crs_file` (including the default ones) are considered.

repint Representative wavelength parameterization for integrated irradiances and heating rate calculations, available options may be selected using `repint_option`.

kato Kato et al. (1999) correlated-k distribution, shortwave; based on HITRAN 96. Please note that the bands above 2.5 micrometer are not very reliable which, however, this has only little impact on integrated shortwave radiation.

kato2 Kato et al. (1999), shortwave; optimized version (Seiji Kato, personal communication, 2003); please note that `kato2` only has 148 subbands (that is, calls to the `rte_solver`) compared to 575 for `kato` which translates to a increase in computational speed by up to a factor of 4 with only little increase in uncertainty. The absorption data are based on HITRAN 2000. Please note that the bands above 2.5 micrometer are not very reliable which, however, this has only little impact on integrated shortwave radiation.

kato2andwandji Similar to `kato2`, but the UV bands #3 and #4 use the improved parameterization by Wandji Nyamsi et al. (2015).

kato2.96 Kato et al. (1999), shortwave; optimized version (Seiji Kato, personal communication, 2003); similar to `kato2` but based on HITRAN96. Please note that the bands above 2.5 micrometer are not very reliable which, however, has only little impact on integrated shortwave radiation.

fu Fu and Liou (1992, 1993), shortwave and longwave; fast parameterization, developed for climate models.

avhrr_kratz Kratz and Varanasi (1995), AVHRR instrument channels

lowtran Gas absorption parameterization from LOWTRAN; code adopted from SBDART (Ricchiazzi et al., 1998); please see the section on "Spectral resolution".

sbdart Identical to LOWTRAN.

If `mol_abs_param` kato/kato2/kato2.96/fu/avhrr_kratz is specified, the extraterrestrial flux is taken from internally defined files specific for each parameterization, not from `source solar file`. The output is the integrated irradiance for each band. To get e.g. integrated shortwave irradiance, simply add all bands of the Kato et al. (1999) or the Fu and Liou (1992, 1993) parameterization. The five AVHRR channels are weighted sums of the libRadtran output. Examples how to integrate the output in

the avhrr_kratz case are included in the *uvspec* self check which is initiated with make check.

mol_file

Specify density profiles (or matrix, see below) of various trace gases to be included in the radiative transfer calculation.

```
mol_file gas_species filename [unit]
```

At the moment following gas_species are included: ozone (O3), nitrogen dioxide (NO2), water vapor (H2O), bromine oxide (BRO), chlorine dioxide (OCLO), formaldehyde (HCHO), carbon dioxide (CO2), sulphur dioxide (SO2), oxygen (O2), the oxygen dimer (O4), methane (CH4), nitrous oxide (N20), carbon monoxide (CO), and nitrogen (N2). The gas species is identified by their abbrevations given in the parenthesis above.

The model expects a density file with two columns:

1 Altitude above sea level in km.

2 The density of trace gas [in the specified unit]

The altitude grid may be different from that in atmosphere_file. All densities inside the range of the mol_file are replaced. For all other altitudes the values from the atmosphere_file are used. If the density is specified as -1 at a level, the value from atmosphere_file is used. Altitude ranges not covered by the atmosphere_file are ignored.

unit is an optional argument to define the unit of the density. The profiles can be given in particles per cm^3 (cm_3), in particles per m^3 (m_3), as volume mixing ratio (vmr), as mass mixing ratio (mmr), or as relative humidity (rh) (only for water). The default for unit is cm^{-3}.

To scale the profile to a total column value use mol_modify.

For airmass factor calculations it is for some species necessary to account for the variation of the profile with sza. This may be accomplished by specifying a mol_file in the following format:

```
 0.0 SZA1 SZA2 ...
z(1) dens(1,1) ...
z(2) .   .
.   .   .
```

where z(i) are the altitude levels above sea level in km, SZA is the solar zenith angle in degrees, and dens is the density [in the specified unit] of the trace gases as function of solar zenith angle and altitude. The matrix may only be specified for one species. It may however be combined with profiles of other species. A density matrix can only be used in connection with rte_solver sdisort!

mol_modify

Set the total column of a density profile. The column is integrated between the user-defined altitude and TOA (top of atmosphere). The syntax is

```
mol_modify species column unit
```

where `species` is one of O3, O2, H2O, CO2, NO2, BRO, OCLO, HCHO, O4, SO2, CH4, N2O, CO, or N2, see also `mol_file`. The second argument is the total column value, and the third argument is the unit, in which the column is given. The unit can be DU (Dobson units), CM_2 (molecules/cm^2) or MM.

Please note that the unit MM is only valid for species H2O and specifies the precipitable water in kg / m2 (which is approximately 1mm).The water vapor profile is scaled accordingly. The precipitable water is integrated from the user-defined `altitude` to TOA (top of atmosphere).

The default units are DU for O3, and CM_2 for all other gases. It is possible to have several `mol_modify` commands in the input file (maximum one per species). The following sets the NO_2 total column to 1.2 DU.

```
mol_modify NO2 1.2 DU
```

mol_tau_file

Location of molecular scattering or absorption optical depth file.

```
mol_tau_file sca/abs filename
```

sca

Usually, the Rayleigh scattering cross section is calculated from the air pressure provided in `atmosphere_file` (scaled with `pressure`). Use this parameter only if you really want to specify the optical depth directly (e.g. for a model intercomparison). The optical thickness profile may be either monochromatic or spectral.

abs

Usually, molecular absorption is calculated from trace gas concentrations provided in `atmosphere_file` (scaled with `mol_modify O3`, etc.). Use this option only if you want to specify the optical depth directly (e.g. for a model intercomparison) or for a line-by-line calculation. If a spectral `mol_tau_file` is specified, the wavelength grid defined there is used as the internal wavelength grid for the radiative transfer calculation, if not defined otherwise with `wavelength_grid_file`.

The file can be either of the following three formats:

Monochromatic

Column 1 is the altitude in km Column 2 is the absorption optical depth of each layer.

Spectral, ASCII

The first line contains the level altitudes in decreasing order; the following lines

contain the wavelength [nm] in the first column and then the absorption optical depths of each layer.

Spectral, netcdf
An example is available at the libRadtran homepage, the file `UVSPEC.O2A.afglms.cdf` is a line-by-line spectrum of the oxygen A-Band around 760nm, calculated for the mid-latitude summer atmosphere. The advantage of netcdf compared to ASCII is that it is much faster to read, and that the file is a self-contained, including data and a description of the variables and arrays. It is therefore particularly useful for line-by-line calculations where usually many spectral data points are involved.

Comments start with `#`. Empty lines are ignored.

no2_column_du
Obsolete, use `mol_modify` instead.

no2_column_moleccm-2
Obsolete, use `mol_modify` instead.

no_absorption
Switch off absorption. Please note that this option simply sets the absorption optical thickness to 0.

```
no_absorption [name]
```

If `name` is not set, all absorption (molecular, aerosol, cloud, ice cloud, and any profile) is switched off.

If used together with `xxx_modify set tau` this might be a bit confusing but probably the most logical way. E.g. when using `aerosol_default` and `aerosol_modify set tau 1`, the aerosol optical thickness is set to 1, with 0.940539 scattering and 0.059461 absorption. If `no_absorption` is added, the absorption optical thickness is set to 0 while the scattering optical thickness is preserved at 0.940539 (even though 1 was specified by the user). We find this the most logical solution of the problem because by switching `no_absorption` off and on one tests the effect of the absorber in an isolated way, rather than mixing absorption and scattering. The same is true for water and ice clouds. Note, that thermal emission of molecules is also switched off.

Possible choises for the optional argument `name` are:

mol Switch off molecular absorption.

no_scattering
Switch scattering off for 1D profiles.

```
no_scattering [name]
```

If `name` is not set, all scattering (molecular, aerosol, cloud, ice cloud, and any profile) is switched off.

Possible choises for the optional argument `name` are:

mol Switch off molecular scattering.

aer Switch off scattering by aerosols.

wc Switch off scattering by water clouds.

ic Switch off scattering by ice clouds.

profile Switch off scattering by any profile defined in `profile typename`.

number_of_streams

Number of streams used to solve the radiative transfer equation.

```
number_of_streams value
```

Default is 6 for fluxes and 16 for radiances. (For `rte_solver fdisort1`, `fdisort2` and `disort` only even number of streams are possible.)

output_file

```
output_file filename
```

uvspec output will be written to `filename`. The format can be set by the option `output_format` (default is ascii).

output_format

```
output_format format
```

where `format` is either `ascii` (default) or `flexstor`. Note that `flexstor` does not currently work when `umu` and/or `phi` is specified. There is also the possibility to write uvspec simulation results to an existing netCDF file. For that `format` must be `netCDF` and the option `output_file` must be given and point to a file that contains a lat/lon/time grid. If `format` is set to `sat picture` then `output_file` must be given and point to a NetCDF-File that contains a pixel x/pixel y/time grid.

output_process

Decide how the output from `uvspec` is processed:

```
output_process type
```

where type is one of

sum

Sum output over wavelength. Useful in combination with the `mol_abs_param` option (`kato`, `kato2`, `kato2.96`, `Fu`, `avhrr_kratz`). In case of `mol_abs_param reptran`, the units are automatically converted to `per_band` before summation.

integrate
Integrate output over wavelength for solar and over wavenumber for thermal simulations. Useful for spectral calculations, `mol_abs_param lowtran` and `reptran`.

per_nm
Output is given in W/(m^2 nm) or mW/(m^2 nm) (W or mW is determined by the extraterrestrial spectrum.)

per_cm-1
Output is given in W/(m^2 cm^{-1}) or mW/(m^2 cm^{-1}).

per_band
Output is given in W/m^2 or mW/m^2 per correlated-k or reptran band. (This option can not be used for spectral calculations and `mol_abs_param` LOWTRAN in the solar range.)

rgb
Output is given as sRGB values computed from spectral radiances. Color channels are correspond to the three output wavelengths. The spectrum is converted to the values in XYZ-colorspace, which is further converted to sRGB. Possible negative RGB-values are constrained (desaturated) before norming to the maximum value and applying gamma correction. The conversion corresponds to the sRGB standard IEC 61966-2-1:1999 to the best of our knwoledge. Especially useful with `rte_solver montecarlo` and `mc_panorama` or `rte_solver disort` with `phi umu` grid.

rgb_raw
Computes sRGB values like `rgb` but does not constrain, norm and gamma correct. Allows users to do this on their own, e.g. to assure equal dynamic range for a series of images by norming to a common value. Python code for manual posprocessing (desaturation/constrain, norm and gamma correction) can be found as comment in `examples/UVSPEC_MC_RGB_PANORAMA_FILE.INP`.

none
No processing - output spectral information (default).

output_quantity
Convert radiances / irradiances to equivalent output quantity.

```
output_quantity quantity
```

where `quantity` can be one of the following:

brightness
Convert radiances / irradiances to equivalent brightness temperatures.

reflectivity
Calculate transmission / reflectivity instead of absolute quantities. For irradiances / actinic fluxes the transmission T is defined as

$$T = \frac{E}{E_0 \cos\theta} \tag{6.7}$$

where E is the irradiance / actinic flux, E_0 is the extraterrestrial flux, and θ is the solar zenith angle. The reflectivity R is defined as

$$R = \frac{\pi \cdot L}{E_0 \cos\theta} \tag{6.8}$$

where L is the radiance, E_0 is the extraterrestrial flux, and θ is the solar zenith angle. Obviously, reflectivities do not depend on Sun-Earth distance. Please note the difference to `transmittance`.

transmittance
Calculate transmittance / reflectance instead of absolute quantities. That is, set the extraterrestrial irradiance to 1 and do not correct for Sun-Earth distance:

$$T = \frac{E}{E_0} \tag{6.9}$$

where E is the irradiance / actinic flux / radiance and E_0 is the extraterrestrial flux. Please note the difference to `reflectivity`.

output_user
User defined output. Here the user may specify the columns desired for output.

```
output_user format
```

where `format` is one or more of the following.

lambda
Wavelength in nm.

wavenumber
Wave number in cm^{-1}.

sza
solar zenith angle

zout
Output altitude in km.

edir, eglo, edn, eup, enet, esum
The direct, global, diffuse downward, and diffuse upward irradiance. Net is global - upward, sum is global + upward.

uu
Radiances: uu(umu(0),phi(0)) ... uu(umu(0),phi(m)) ... uu(umu(n),phi(0)) ... uu(umu(n),phi(m))

fdir, fglo, fdn, fup, f
The direct, global, diffuse downward, diffuse upward, and total actinic flux.

uavgdir, uavgglo, uavgdn, uavgup, uavg
The Direct, global, diffuse downward, diffuse upward, and total diffuse mean intensity (= actinic flux / 4π).

spher_alb
Spherical albedo of the complete atmosphere.

albedo
Albedo.

heat
Heating rate in K/day.

It is also possible to gain some information about the atmosphere and the clouds:

p
pressure [hPa], ,

T, T_d
temperature [K], dewpoint temperature [K]

T_sur
surface temperature [K]

theta
potential temperature [K]

theta_e
equivalent potential temperature [K]

n_xxx
number density of the gas xxx [cm^{-3}]

rho_xxx
mass density of the gas xxx [kg/m^3]

mmr_xxx
mass mixing ratio of the gas xxx [kg/kg]

vmr_xxx
volume mixing ratio of the gas xxx [m^3/m^3]

rh
relative humidity over water [percent]

rh_ice
relative humidity over ice [percent]

c_p
specific heat capacity of the air (humidity and temperature dependent)

CLWC
cloud liquid water content [kg/kg]

CLWD
cloud liquid water density [g/m^3]

CIWC
cloud ice water content [kg/kg]

CIWD
cloud ice water density [g/m^3]

TCC
total cloud cover [0-1]

where xxx is one of AIR, O3, O2, H2O, CO2, NO2, BRO, OCLO, HCHO, or O4.

Default output is

```
 output_user lambda lambda, edir, edn, eup, uavgdir, uavgdn,
uavgup
```

for fdisort1, sdisort, and spsdisort, whereas the default for twostr is

```
 output_user lambda, edir, edn, eup, uavg.
```

The lines containing radiances are not affected.

ozone_column

Obsolete, use mol_modify instead.

phi

Azimuth output angles (in degrees) in increasing order.

```
 phi values
```

The radiance is output at phi and umu.

- Sensor in the North (looking South): 0 deg
- Sensor in the East (looking West): 90 deg
- Sensor in the South (looking North): 180 deg
- Sensor in the West (looking East): 270 deg

For all one-dimensional solvers the absolute azimuth does not matter, but only the relative azimuth phi-phi0.

phi0

Azimuth angle of the sun (0 to 360 degrees).

```
phi0 value
```

- Sun in the South: 0 degrees
- Sun in the West: 90 degrees
- Sun in the North: 180 degrees
- Sun in the East: 270 degrees

For all one-dimensional solvers the absolute azimuth does not matter, but only the relative azimuth phi-phi0.

pressure

The surface pressure (at the user-defined altitude) in hPa.

```
 pressure value
```

The pressure profile as well as air, O2 and CO2 density profiles are scaled accordingly.

pressure_out

Specify the output levels in pressure coordinates. The syntax is

```
pressure_out p1 p2 ...
```

where 'p1 p2 ...' are the output levels in hPa. The pressure output levels must be sorted in decreasing order. Output pressure levels must be within the range defined in the atmosphere_file. You can also use toa for top of atmosphere and sur for surface altitude and cpt for cold point tropopause.

print_disort_info

Specify one or more integers between 1 and 7.

```
print_disort_info value
```

Print various disort input and output in disorts own format. See libsrc_f/DISORT2.doc for more information. **Warning:** Produces a lot of output.

profile_file

Define file containing properties of clouds, aerosols, hydrometeors, etc. This option is a generalization of the options wc_file and ic_file.

Usage:

```
profile_file typename type file
```

typename describes the name of the profile; typically this describes what kind of particles are dealt with here. Examples are wc (water clouds), ic (ice clouds), aer (aerosols), drizzle. The typename is needed to refer to this profile when using other options, such as profile_properties. Note that typename "wc" and "ic" have special effects (i.e. default properties, and "ic" properties are not allowed with "wc" files, and vice versa).

type defines the file type, which is identical to wc_file type. Please refer to wc_file for choises of type and a detailed description on the file structures.

profile_modify

Modify profile optical properties.

```
profile typename variable scale/set value
```

typename describes the name of the profile; it must be identical to the one defined in profile_file.

This option is identical to `wc_modify`. Please refer to `wc_modify` for a detailed description of `variable`.

profile_properties

Define how liquid/ice water content/mass concentration and effective particle radius are translated to optical properties for profile `typename`. This option is a generalization of the options `wc_properties` and `ic_properties`.

Usage:

```
profile_properties typename property [interpolate]
```

`typename` describes the name of the profile; it must be identical to the one defined in `profile_file`.

Please refer to `wc_properties` and `ic_properties` for possible choices for `property`.

pseudospherical

Invokes pseudo-spherical geometry in disort/twostr. Default is plane-parallel.

quiet

If specified, informative messages are turned off. See also `verbose`.

radiosonde

This option allows to change the temperature and pressure profile, and optionally to specify one or more density profiles. The entry in the input file looks like this:

```
radiosonde filename [gas_species] [unit] ...
```

Currently the following gas_species are included: ozone (O3), nitrogen dioxide (NO2), water vapor (H2O), bromine oxide (BRO), chlorine dioxide (OCLO), formaldehyde (HCHO), carbon dioxide (CO2), sulphur dioxide (SO2), and the oxygen dimer (O4). Each gas species is identified by its abbrevations given in parentheses above. Unit is an optional argument to defines the unit of the density. The profiles can be given in particles per cm^3 (CM-3), in particles per m^3 (M-3), as volume mixing ratio (VMR), as mass mixing ratio in kg/kg (MMR), or as relative humidity (RH) (only for water). The default unit is RH for water vapour, MMR for ozone, and CM3 for all other gases. The radiosonde file must have (2 + number of gases) columns:

1 pressure in hPa

2 temperature in Kelvin

3, 4, ... density of trace gas in the specified unit

A new z-grid will be calculated, starting at `altitude` and assuming a linear temperature variation between levels. The air density will be recalculated according to the ideal gas law, and the density of the well mixed gases O2 and CO2 will be

scaled accordingly. The atmospheric data above the radiosonde data is taken from the `atmosphere_file` level by level, starting at the first pressure level above the radiosonde data. The z-grid of the `atmosphere_file` in this height region is shifted accordingly. Also if the density in the radiosonde file is specified as -1 at a level, the value from the `atmosphere_file` is used. Possible calls are

```
radiosonde ../examples/radiosonde.dat
```

just in order to change the temperature and pressure profile, or

```
radiosonde ../examples/radiosonde2.dat H2O RH O3 MMR NO2
```

where water vapour density will be given as relative humidity, ozone as mass mixing ratio, and NO2 in cm^{-3} (default).

radiosonde_levels_only

The atmosphere considered in the simulation has the same height range as the data in the `radiosonde`-file. No further levels are added above those. This option has only an effect in combination with `radiosonde`.

raman

```
raman [original]
```

The `raman` option includes single order rotational Raman scattering in the calculation. The solution treats Raman as a perturbation similar to the approaches of Vountas et al. (1998) and Spurr et al. (2008).

The `raman` option may only be used for spectral calculation.

The disort radiative transfer solver with a general source is needed to solve the radiative transfer equation including Raman scattering. This solver is automagically invoked when specifying the `raman` option. It is thus not neccessary to set the `rte_solver`.

The `raman` option is optimized with respect to speed. The optimized implementation should be just as accurate as the original version. To use the original version invode `raman original`. With the optional argument `original` each wavelength is treated individually and is thus accurate, but computationally very expensive.

Please note that while the `raman` option has been extensively tested and verified, it is nevertheless a new option, hence, use it with care.

rayleigh_depol

Rayleigh depolarization factor.

```
rayleigh_depol value
```

The Rayleigh scattering phase function is $p(\mu) = a + b\mu^2$ where $a = 1.5(1 + \mathtt{depol})/(2 + \mathtt{depol})$ and $b = 1.5(1 - \mathtt{depol})/(2 + \mathtt{depol})$.

By default the depolarization is calculated using the expressions from Bodhaine et al. (1999).

refractive_index_pv
Specify refractive index of glass surface of photovoltaic module. This option can be used in combination with `mc_backward_quantity ednpv`.

repint_option
Specify REPINT parameterization.

```
repint_option option_name
```

This option is useful together with 'mol_abs_param reptran int'. Spectrally integrated irradiances are approximated by weighted sums over representative wavelengths which were found by simulated annealing (de Mourgues et al., 2022; Meier, 2022; Gasteiger et al., 2014). The following options are available:

deMourgues10
thermal range, 10 representative wavelengths

deMourgues30
thermal range, 30 representative wavelengths

deMourgues50
thermal range, 50 representative wavelengths

deMourgues100
thermal range, 100 representative wavelengths

reptran_file
Location of the representative wavelengths file.

```
reptran_file file
```

This option is useful together with 'mol_abs_param reptran' and 'mol_abs_param reptran_channel' options, if you want to use your own representative wavelengths parameterization.

reverse_atmosphere
Option for the strong and bold. Reverses the atmospheric input to the radiative transfer solvers. That is, the atmosphere is turned on the head. Yes, that is actually useful for some purposes. If you think you need this contact the author. Otherwise, do not use.

rte_solver
Set the radiative transfer equation solver to be used.

```
rte_solver type
```

If not specified the default `rte_solver` is `disort`. Choices for `type` are

disort
C-version of the disort algorithm, translated from Fortran by Tim Dowling. This is the recommended discrete ordinate code in *libRadtran*. For documentation see `src_f/DISORT2.doc` as well as the papers and the DISORT report at ftp://climate1.gsfc.nasa.gov/wiscombe/Multiple_Scatt/. The intensity correction can be performed according to Nakajima and Tanaka (1988) using `disort_intcor moments` (like in the original code), or with the improvements described in Buras et al. (2011). Can be run in plane-parallel geometry (default) or in pseudo-spherical geometry (using `pseudospherical`).

twostr
C-version of the two–stream radiative transfer solver described by Kylling et al. (1995). Can be run in plane-parallel geometry (default) or in pseudo-spherical geometry (using `pseudospherical`).

fdisort1
The standard plane–parallel disort algorithm by Stamnes et al. (1988), version 1.3 – provided for compatibility reasons. Use only if you have troubles with the default `disort` or for historical reasons. For documentation see `src_f/DISORT.doc` as well as the papers and the DISORT report at ftp://climate1.gsfc.nasa.gov/wiscombe/Multiple_Scatt/. To optimize for computational time and memory, please adjust the parameters in `src_f/DISORT.MXD` for your application and re-compile. For your application please use `rte_solver fdisort2` which is the advanced version, unless you e.g. want to explore how a specific feature of `fdisort2` (e.g. the Nakajima and Tanaka (1988) intensity correction) improves the `fdisort1` result.

fdisort2
Version 2 of the Fortran algorithm disort – provided for compatibility reasons. Use only if you have troubles with the default `disort` or for historical reasons. For documentation see `src_f/DISORT2.doc` as well as the papers and the DISORT report at ftp://climate1.gsfc.nasa.gov/wiscombe/Multiple_Scatt/ `fdisort2` has several improvements compared to its 'ancestor' `fdisort1` (version 1.3). To optimize for computational time and memory, please adjust the parameters in `src_f/DISORT.MXD` for your application and re-compile. Note! `fdisort2` is a new version of the original disort code which was implemented in summer 2009. It uses phase functions to calculate the intensity corrections by Nakajima and Tanaka (1988) instead of Legendre moments. Hence it needs cloud properties files which contain the phase functions. It is still possible to use the old version of disort, you need to specify `disort_intcor moments`.

sdisort
Pseudospherical disort as described by Dahlback and Stamnes (1991). Double precision version. To optimize for computational time and memory, please adjust the parameters in `src_f/DISORT.MXD` for your application and re-compile.

spsdisort

Pseudospherical disort as described by Dahlback and Stamnes (1991), single precision version. **Warning:** it is not recommended to use `spsdisort` for really large solar zenith angles nor for cloudy conditions. For large optical thickness it is numerically unstable and may produce wrong results. To optimize for computational time and memory, please adjust the parameters in `src_f/DISORT.MXD` for your application and re-compile.

ftwostr
Original Fortran-version of the two–stream radiative transfer solver described by Kylling et al. (1995), in pseudo-spherical geometry.

rodents
Delta-Eddington two–stream code (RObert's Delta-EddingtoN Two-Stream), plane-parallel.

schwarzschild
Solver for the thermal spectral region which neglects scattering and calculates irradiances by solving the Schwarzschild equation. You may set the number of angular streams with option `schwarzschild_streams`.

twomaxrnd
Delta-Eddington two–stream solver with Maximum-Random-Overlap according to Zdunkowski et al. (2007) by Nina Crnivec. As inputs, a `wc_file 1D` and/or a `ic_file 1D` are required, plus a `cloud_fraction_file`. The same cloud fraction is used for water and ice clouds. `zout_interpolate` is activated automatically. See Črnivec and Mayer (2019) for more details.

twomaxrnd3C
Delta-Eddington two–stream solver with Maximum-Random-Overlap according to Zdunkowski et al. by Nina Crnivec. In addition to `twomaxrnd` "tripleclouds" by Shonk and Hogan (2008) is considered. A `cloud_fraction_file` has to be specified as well as two cloudy columns, defined as profiles wcn (optically thiN) and wck (optically thicK clouds), e.g. `profile_file wcn 1D ./wcn.dat.` `zout_interpolate` is activated automatically.See Črnivec and Mayer (2020), in particular appendix A.

twomaxrnd3C_scale_cf
Scaling factor for cloud fraction split.

sslidar
A simple single scattering lidar simulator by Robert Buras.

sos
A scalar pseudospherical succesive orders of scattering code. Works for solar zenith angles smaller than 90 degrees. Can calculate azimuthally averaged radiances. Set `sos_nscat` to specify the order of scattering.

montecarlo
The MYSTIC Monte Carlo code. Monte Carlo is the method of choice (1) for horizontally inhomogeneous problems; (2) whenever polarization is involved; (3) for applications where spherical geometry plays a role; and (4) whenever sharp features of the scattering phase function play a role, like for the calculation of the backscatter glory or the aureole.

mystic
Same as `montecarlo`.

tzs
TZS stands for "thermal, zero scattering" and is a very fast analytical solution for the special case of thermal emission in a non-scattering atmosphere. Please note that TZS does only radiance calculations at top of the atmosphere. "Blackbody clouds" may be included using the option `tzs_cloud_top_height`.

sss
SSS stands for "solar, single scattering" and is an analytical single scattering approximation which might be reasonable for an optically thin atmosphere. Please note that SSS does only radiance calculations at top of the atmosphere. This is an experimental solver - be careful!

null
The NULL solver does not solve the radiative transfer equation. However, it sets up the optical properties, and does the post-processing; useful if you are either interested in the overhead time required by a particular model input or if you are simply interested in the optical properties, as output by `verbose`.

Default: `disort`

schwarzschild_streams
Number of zenith angles to use when integration radiances.

sdisort
Specify sdisort values. This option is only relevant for `rte_solver sdisort`.

```
sdisort nscat value
```

Set the order of scattering. If `value` is set to 1 `sdisort` will run in single scattering mode while if set to 2, `sdisort` runs in full multiple scattering mode. Default is 2 for `rte_solver sdisort`.

```
sdisort nrefrac value
```

Include refraction where `value` has the meaning

0 No refraction, default.

1 Refraction included using fast, but harsh method.

2 Refraction included using slow, but accurate method.

If refraction is included also set parameter `refraction_file`.

slit_function_file
If specified, the calculated spectrum is convolved with the function found in the `slit_function_file`.

```
slit_function_file file
```

The file must contain two columns. Column 1 is the wavelength, in nm, and relative to the center wavelength. Column 2 is the corresponding slit function value. It must be unity at the maximum. The wavelength steps in the slit function file must be equidistant. Comments start with `#`. Empty lines are ignored. Please note that prior to convolution the spectrum is interpolated to the wavelength steps of the slit function. For this reason, make sure that the resolution of the slit function is high enough even if the slit function is e.g. a simple triangle which could in principle be described with 3 grid points. For an example see `examples/TRI_SLIT.DAT` and the `make_slitfunction` tool.

source

Set the radiation source type

```
source type
```

where `type` is either `solar` or `thermal`. Solar radiation is per default output in W/(m2 nm) if no `mol_abs_param` is specified or `mol_abs_param` options `crs`, `lowtran`, or `reptran` are specified. For all other `mol_abs_param` options the output is integrated over the wavelength band. Thermal radiation is per default output in W/(m2 cm-1), if REPTRAN is used or the bandwidth is equal to 1 cm-1 (default for `mol_abs_param lowtran`). Otherwise the output is the integrated flux over the wavenumber interval specified by `thermal_bandwidth`, `thermal_bands_file`, or by the `mol_abs_param` option (`kato`, `kato2`, `kato2.96`, `fu`, or `avhrr_kratz`).

```
source type [file] [unit]
```

The second argument `file` specifies the location of file holding the extraterrestrial spectrum. In general, `file` is required for solar calculations if `mol_abs_param` is not used. `file` is ignored if `mol_abs_param` other than `lowtran` oder `reptran` is specified.

The file must contain two columns. Column 1 is the wavelength in nm, and column 2 the corresponding extraterrestrial flux. The user may freely use any units he/she wants for the extraterrestrial flux. The wavelength specified grid defines the wavelength resolution at which results are returned. However, the wavelength range is determined by `wavelength`. `file` may be omitted for thermal radiation calculations (`source thermal`) as well as `output_quantity transmittance` and `output_quantity reflectivity` calculations. If omitted, the output resolution equals the internal wavelength grid which the model chooses for the radiative transfer calculation. Comments start with `#`. Empty lines are ignored.

For some purposes it is useful to tell libRadtran the units of the spectrum. This can be done with the optional third argument. Possible choises for `unit` are `per_nm`, `per_cm-1` or `per_band`. If `unit` is set to `per_nm` libRadtran assumes that the unit of the spectrum is W/(m2 nm), if set to `per_cm-1` it assumes W/(m2 cm-1).

spline

```
spline lambda_0 lambda_1 lambda_step
```

Spline interpolate the calculated spectrum between wavelengths `lambda_0` and `lambda_1` in steps of `lambda_step`, in nm. Specified as e.g.

```
spline 290.  365.  0.5
```

Here, the calculated spectrum is interpolated to wavelengths 290.0, 290.5, 291.0, ..., 364.5, 365.0. For interpolation to arbitrary wavelengths use `spline_file`. The specified wavelength interval must be within the one specified by `wavelength`.

spline_file

Spline interpolate to arbitrary wavelengths, in nm, given as a single column in file `spline_file`.

```
spline_file file
```

The specified wavelengths must be within the range specified by `wavelength`. Comments start with `#`. Empty lines are ignored.

sslidar

Set single scattering lidar parameters (`rte_solver sslidar`).

```
sslidar variable value
```

`variable` can be one of the following:

area Set area of single scattering lidar in units of square meters (default: 1.0)

E0 Set Laser pulse energy for single scattering lidar in units of (default: 0.1) Joule (You can also use a `source solar file` instead... not yet implemented.)

eff Set lidar efficiency for single scattering lidar (default: 0.5)

position Set lidar position for single scattering lidar in units of km (default: 0.0)

range Set lidar range bin width for single scattering lidar in units of km (default: 0.1)

sslidar_nranges

Set number of range bins for single scattering lidar (solver `sslidar`). Default is 100.

sslidar_polarisation

Turn on polarisation measurement for lidar (solver `sslidar`). Default is without polarisation.

sur_temperature

Surface temperature, used for thermal infrared calculations.

```
sur_temperature value
```

If not specified, the temperature of the lowest atmospheric level is used as surface temperature.

surface_type_map

Specify a surface type map, which is used in combinition with `albedo_library`, `latitude`, and `longitude` in order to select the surface type relevant for the simulation. No pixel interpolation is done. The format of the call is:

```
surface_type_map file [variable_name]
```

where `file` is the location of the surface type map file. The map is expected to be in *netCDF* format. The file must contain the variables `double lat(nlat)`, `double lon(nlon)`, and `byte brdf_rpv_type (nlat, nlon)`. If the name of the surface type variable is different, the optional argument can be used in order to specify the variable name. For format specification see also `data/albedo/IGBP_map/SURFACE_TYPE_IGBP_10min.cdf`.

For using the IGBP map, the call is `surface_type_map IGBP`. This map has a resolution of 10 minutes and contains the surface types 1 to 18 defined in the `albedo_library IGBP`. Fresh snow and sea ice are not included, as their extent is too variable. Attention: That implies e.g. that the Arctic is considered ocean_water and not sea_ice!

Locations on the pixel boundaries are interpreted as the pixel northward and eastward respectively. E.g. location 0 N, 0 E is interpreted like the pixel ranging from 0 to 10min North and from 0 to 10min East.

sza

The solar zenith angle (degrees).

```
sza value
```

The default solar zenith angle is 0.

sza_file

Location of solar zenith angle file for wavelength-dependent solar zenith angle.

```
sza_file file
```

This option is useful if you want to simulate an instrument which scans so slowly that the solar zenith angle may change significantly during the wavelength scan. The file must have two or three columns. Column 1 is the wavelength, in nm, and column 2 the corresponding solar zenith angle. Optionally the third column may contain the corresponding solar azimuth angle. The solar azimuth angle is only needed when calculating radiances. The wavelength grid may be freely set. The solar zenith and azimuth angle will be interpolated to the wavelength grid used for the radiation calculation. Comments start with `#`. Empty lines are ignored.

thermal_bands_file

File with the center wavelengths and the wavelength band intervals to be used for calculations in the thermal range.

```
thermal_bands_file file
```

The following three columns are expected: center (or reference) wavelength, lower wavelength limit, upper wavelength limit [nm]. `thermal_bands_file` defines the wavelength grid for the radiative transfer calculation. The RTE solver is called for each of the wavelengths in the first column. The atmospheric (scattering, absorption, etc) properties are also evaluated at these wavelengths. For thermal radiation calculations, the Planck function is integrated over the wavelength bands defined in the second and third columns. The result will therefore be a band-integrated irradiance which does only make sense when the `source solar file` grid equals the `thermal_bands_file` grid.

thermal_bandwidth

Specify a constant bandwidth in cm-1 for thermal calculations.

```
thermal_bandwidth value
```

The default is 1 cm-1. This option is ignored if used together with `mol_abs_param kato/kato2/kato2.96/fu/avhrr_kratz`.

time

Specifies the time to simulate.

```
time YYYY MM DD hh mm ss
```

where `YYYY` is the year, `MM` the month, `DD` the day, `hh` the hour, `mm` the minute, `ss` the second in UTC. The time information will be used for a couple of things:

`time` in combination with `latitude`, `longitude`, and any `map`-option is used to select the location where to read the input data.

`time` is used to correct extraterrestrial irradiance for the Sun-Earth distance with the day of year. If not given, the Earth-Sun distance is 1 AU (i.e. equinox distance).

`time` in combination with `latitude` and `longitude` is used to calculate the solar zenith angle if no `sza` is specified.

`time` in combination with `latitude` and `longitude` is used to choose a suitable default atmosphere file, if no `atmosphere_file` is specified.

`time` in combination with an `ECMWF_atmosphere_file` is used to choose a date in the ECMWF input file.

twomaxrnd3C_scale_cf

Scale factor for cloud fraction split for radiative transfer solver `twomaxrnc3C`.

tzs_cloud_top_height

Define cloud top height of "blackbody clouds" for radiative transfer solver `tzs`.

umu

Cosine of output polar angles in increasing order, starting with negative (downwelling radiance, looking upward) values (if any) and on through positive (upwelling radiance, looking downward) values. Must not be zero.

```
umu values
```

verbose

If specified abundances of informative messages are output to stderr. To make use of this information, you may want to write the standard `uvspec` output to one file and the diagnostic messages to another. To do so, try `(./uvspec < uvspec.inp > uvspec.out) >& verbose.txt` (depending on your shell you might need a slightly different syntax). The irradiances and radiances will be written to `uvspec.out` while all diagnostic messages go into `verbose.txt`. See also `quiet`.

wavelength

Set the wavelength range by specifying first and last wavelength in nm.

```
wavelength lambda_0 lambda_1
```

The default output wavelength grid is that defined in `source solar file`, unless `spline` is specified. Note that the radiative transfer calculations are done on an internal grid which can be influenced with `wavelength_grid_file` or `mol_tau_file abs file`

wavelength_grid_file

Location of single column file that sets the wavelength grid used for the internal transmittance calculations.

```
wavelength_grid_file file
```

The wavelengths must be in nm. Do not use this option unless you know what you are doing. Comments start with #. Empty lines are ignored.

wavelength_index

Set the wavelengths to be selected. To be used together with predefined wavelength grids, such as `wavelength_grid_file`, `mol_tau_file abs file` and particularly useful in combination with the `mol_abs_param` option where often only a specified number of wavelength bands is required. E.g., in combination with `mol_abs_param AVHRR_KRATZ`, `wavelength_index 15 15` will select wavelength index 15 which corresponds to channel 4, or `wavelength_index 10 14` will select those bands required for channel 3. Indices start from 1.

wc_file

Location of file defining water cloud properties.

```
wc_file type file
```

type defines the file type, which can be one of the following:

1D Location of file defining one-dimensional profile.

The file must contain three columns: Column 1 is the altitude in km, column 2 the liquid water content (LWC) in grams per cubic meter, and column 3 the effective droplet radius in micrometer. Empty lines are ignored. Comments start with #. Note that the definition of cloud altitudes in wc_file 1D refers to sea level, not to altitude above ground. E.g., when altitude is set to 1.63km, and the first cloud level is defined at 3km, the cloud would start at 1.37km above ground. An example of a water cloud is given in examples/WC.DAT.

Per default the cloud properties are interpreted as layer properties. Before version 1.4 the default was level properties: The optical depth of a layer was calculated using information from the upper and lower levels defining the layer. To switch to the old behaviour, use interpret_as_level. See section 3.3.5 about water clouds for a realistic example how the contents of the wc_file 1D are converted to optical properties.

ipa_files A two-column file, defining water cloud property files (see wc_file 1D) in the first column and the correspoding weights in the second column. The radiative transfer calculation is performed independently for each cloud column and the result is the weighted average of all independent columns. If ic_file ipa_files and wc_file ipa_files are both defined, both must have the same columns in the same order, otherwise uvspec will complain. See examples/UVSPEC_WC_IC_IPA_FILES.INP for an example.

moments A way to specify water cloud extinction coefficient, single scattering albedo, and scattering phase function for each layer.

The file specified by wc_file moments has two columns where column 1 is the altitude in km. The second column is the name of a file which defines the optical properties of the layer starting at the given altitude. The files specified in the second column must have the following format:

Column 1: The wavelength in nm. These wavelengths may be different from those in source solar filename. Optical properties are interpolated to the requested wavelengths.

Column 2: The extinction coefficient of the layer in units km-1.

Column 3: The single scattering albedo of the layer.

Column 4-(nmom+4): The moments of the scattering phase function.

Note that if using the rte_solver disort or rte_solver fdisort2 it makes good sense to make the number of moments larger than number_of_streams because all moments are used in the calculation. For rte_solver fdisort1 the number of moments included in the calculations will be number_of_streams+1. Higher order moments will be ignored for these solvers. Please note that the uppermost line of the wc_file moments denotes simply the top altitude of the uppermost layer. The optical properties of this line are consequently ignored. There are two options for this

line: either an optical property file with zero optical thickness is specified or "NULL" instead.

wc_modify

Modify water cloud optical properties.

```
wc_modify variable scale/set value
```

`variable` can be one of the following parameter:

gg

Modify the water cloud asymmetry factor for all wavelengths and altitudes.

set `value` can be a float between -1.0 and 1.0. Please note that this option is only applied if a Henyey-Greenstein phase function is used but not if an explicit phase function is defined e.g. with `wc_file moments`. It doesn't make sense to modify only the first moment of an explicit phase function. This option is useful only for monochromatic calculations or in wavelength regions where the optical properties of water clouds can be considered constant, e.g. the ultraviolet range.

scale Scale the water cloud asymmetry factor for all wavelengths and altitudes with `value` between 0.0 and 1.0.

ssa

Modify the water cloud single scattering albedo for all wavelengths and altitudes.

set `value` can be a float between 0.0 and 1.0. This option is useful only for monochromatic calculations or in wavelength regions where the optical properties of water clouds can be considered constant, e.g. the ultraviolet range.

scale Scale the water cloud single scattering albedo for all wavelengths and altitudes with `value` between 0.0 and 1.0.

tau

Modify the total water cloud optical thickness.

set Set optical thickness to a constant value for all wavelengths. The optical thickness defined here is the integral from the surface at the user-defined `altitude` to TOA (top of atmosphere). This option is useful only for monochromatic calculations or in wavelength regions where the optical properties of water clouds can be considered constant, e.g. the ultraviolet range.

scale Scale the water cloud optical thickness for all wavelengths and altitudes with `value` between 0.0 and 1000000.0. Also works for 3d clouds.

tau550

Set the water cloud optical thickness at 550nm. The optical thickness defined here is the integral from the surface at the user-defined `altitude` to TOA (top of atmosphere). Other wavelengths are scaled accordingly. Note that this option requires for technical reasons that the wavelength interval defined by `wavelength` does contain 550nm.

```
wc_modify tau550 set value
```

wc_properties

Define how liquid water content and effective radius are translated to optical properties.

```
wc_properties property [interpolate]
```

Possible choices for `property` are:

hu

Parameterization by Hu and Stamnes (1993); this is the default setting. Note that the parameterization is somewhat different for `mol_abs_param FU` than for all other cases because in the latter case the parameterization from the newer (March 2000) Fu and Liou code is used while otherwise the data are taken from the original paper by Hu and Stamnes (1993). Note that this parameterization has been developed to calculate irradiances, hence it is less suitable for radiances. This is due to the use of the Henyey-Greenstein phase function as an approximation of the real Mie phase function.

echam4

Use the very simple two-band parameterization of the ECHAM4 climate model, described in Roeckner et al. (1996); this is probably only meaningful if you want to compare your results with ECHAM4, the two bands are 0.2 - 0.68 micrometer and 0.68 - 4.0 micrometer; within these bands, the optical properties are assumed constant.

mie

Use pre-calculated Mie tables; useful for `mol_abs_param`; the tables are expected in `data_files_path/correlated_k/.../`.
For spectral or pseudo-spectral (`mol_abs_param sbdart`) calculations, a set of pre-calculated tables is also available. For spectral or pseudo-spectral calculations optional argument `interpolate` has to be defined explicitely to initiate the interpolation of the optical properties to the internal wavelength grid. The Mie tables are not part of the standard distribution (because of their large size) but they are freely available from http://www.libradtran.org. This is the correct option to calculate radiances, to be preferred over the Henyey-Greenstein approach of Hu and Stamnes (1993).

filename

Read optical properties from specified filename; file format is as produced by the `mie`-tool of the *libRadtran* package (see `output_user netcdf`).

With the optional argument `interpolate` the water cloud optical properties are interpolated over wavelength; useful for precalculated optical property files. Please note that this option may be extremely memory-consuming because for each internal

wavelength a full set of Legendre moments of the phase function is stored (up to several thousands).

write_optical_properties

Write optical properties to netCDF file as used within libRadtran for a given input file. Atmosphere is set up according to the input file, but the actual RTE solver call is omitted. This option is experimental and not yet tested for all solvers and combinations of options. Due to the internal structure, currently one optical property file is written per wavelength or band.

z_interpolate

zout

This option is used to specify the output altitudes in km *above surface altitude*. One or more altitudes may be specified in increasing magnitude.

```
zout 0 1 2 3 4 5 ...
```

Output altitudes must be within the range defined in the `atmosphere_file`. Note that `zout` does not restructure the atmosphere model. Hence, if you specify `zout 0.730` and have your atmosphere model in `atmosphere_file` go all the way down to sea level, i.e. 0.0km., output is presented at 0.730km and calculations performed with an atmosphere between 0.0 and 0.730 km (and above of course). If you want calculations done for e.g. an elevated site you have to restructure the atmosphere model and make sure it stops at the appropriate altitude. This you may either due by editing the atmosphere file or by using `altitude`. You can also use `toa` for `top of atmosphere` and `sur` for `surface altitude` and `cpt` for `cold point tropopause`.

Instead of specifying the altitudes in km, it is also possible to use keywords as argument for this option. Possible keywords are `atm_levels`, `all_levels`, `model_levels`, `model_layers`, and `model_levels_and_layers`. For `atm_levels`, all levels from the `atmosphere_file` are used as output levels. For `all_levels`, all levels (including levels from `atmosphere_file`, `mol_file`, cloud files, `altitude` options) are used as output levels. For `model_levels`, `model_layers`, `model_levels_and_layers` the levels, layers, or both from the `ECMWF_atmosphere_file` are used as output level. Usage e.g.:

```
zout model_levels [nlev_max]
```

With the optional argument `nlev_max` the user may specify the number of zout layers from the ground.

zout_interpolate

The z-grid of optical properties is determined by the `atmosphere_file`, and, if specified, by other profile files like `mol_file`, `rh_file`, or `refractive_index_file`. Additional levels might be introduced by the

zout option and the second argument of the altitude option. By default (if zout_interpolate is not specified) levels introduced by the zout option will not affect the optical property profiles, that is, the optical properties are constant within the layers specified by the atmosphere_file and profile files. If zout_interpolate is specified, the atmospheric profiles (trace-gases, temperature ...) are interpolated to the levels introduced by zout, and optical properties are determined from the interpolated atmospheric properties. If heating_rate, rte_solver rodents, rte_solver twostrebe, rte_solver twomaxrnd, rte_solver twomaxrnd3C, rte_solver dynamic_twostream is specified, zout_interpolate will also be automatically activated. zout_interpolate generally causes smoother variation of the optical properties.

zout_sea

like zout, but *above sea surface*

6.2 Tool for Mie calculations - `mie`

The various input parameters of the `mie` tool are described in the following.

accuracy_phase
Accuracy of the phase function values in the netcdf output. Default value is 0.01 (1 percent).

aerosol_type
With this option Mie calculations are performed for the specified aerosol type.

```
aerosol_type type
```

The aerosol properties (refractive index, size distribution, density, humidity) are taken from the OPAC database (Hess et al., 1998) Possible values for `type` are

inso
Water insoluble aerosol consists mostly of soil particles with a certain amount of organic material.

waso
Water soluble aerosol originates from gas to particle conversion and consists of various types of sulfates, nitrates, and other, also organic water-soluble substances.

soot
Soot is absorbing black carbon, which is not soluble in water. In reality soot particles have a chain-like character, which of course is not accounted for in Mie calculations of optical properties. The optical properties are calculated assuming many very small spherical particles.

ssam
Sea salt particles consist of the various kinds of salt contained in seawater. The different modes are given to allow for a different wind-speed-dependant increase of particle number for particles of different size. This aerosol type represents the accumulation mode.

sscm
Sea salt particles (coarse mode).

minm
Mineral aerosol or desert dust is produced in arid regions. It consists of a mixture of quartz and clay minerals and is modeled with three modes to allow to consider increasing relative amount of large particles for increased turbidity. This aerosol type represents the nucleation mode.

miam
Mineral aerosol (accumulation mode).

micm
Mineral aerosol (coarse mode).

mitr
Mineral transported is used to describe desert dust that is transported over long distances with a reduced amount of large particles.

suso
The sulfate component is used to describe the amount of sulfate found in the Antarctic aerosol. This component is not suited to describe antropogenic sulfate aerosols that are included in the water-soluble component.

alpha_file
Specify various α for gamma or lognormal size distributions (see option `distribution` for the definition of α) in a one column file. In combination with `output_user netcdf`, one netcdf file for each value of α is generated. So far, this option is only included for calculations at one wavelength.

basename
Filename for output of Mie program.

```
basename filebase
```

This option is only used in combination with `output_user netcdf`. The default is wc. for water, ic. for ice, or waso., inso. etc. for OPAC aerosols.

distribution
If specified the effective radius is converted into a size distribution of droplets.

```
distribution distribution_type distribution_parameter
```

where distribution type is one of the two following:

GAMMA
The Gamma distribuition of cloud droplet sizes is

$$n(r) = ar^{\alpha} \exp(-br), \tag{6.10}$$

where α is the distribution parameter given as second argument. (a and b are determined automatically.) The effective radius of the distribution is $r_{\text{eff}} = (\alpha + 3)/b$. A typical value for water clouds is $\alpha = 7$. For ice clouds a typical value is $\alpha = 1$. A large value of α gives close to a monodisperse distribution.

LOGNORMAL
The lognormal distribution of cloud droplet sizes is

$$n(r) = \frac{a}{r} \exp\left(-\frac{1}{2}\left(\frac{\ln(r) - \ln(r_0)}{ln(\sigma)}\right)^2\right), \tag{6.11}$$

where r_0 is the logarithmic mode of the distribution (provided by option `r_eff`) and σ is the standard deviation, which is given by the second argument.

dx_max

This option makes sense in combination with `distribution GAMMA` or `distribution LOGNORMAL`. It can be used to specify the maximum widths of the size distribution bins, which are sampled on a size parameter ($\frac{2\pi r}{\lambda}$) grid. The default value is 0.03 which is not very accurate for small wavelengths. In order to get accurate phase matrices this value should be decreased.

mass_density

Specifies the mass density of the medium.

```
mass_density value
```

Useful in combinition with `refrac user` and `output_user cloudprop`, as the format of `cloudprop` specifies the extinction coefficient per mass and not per volume as usual in this mie program.

mie_program

Specify which Mie program to use:

```
mie_program type
```

where `type` is one of

BH

The Mie scattering program by Bohren and Hoffmann, ftp://ftp.astro.princeton.edu/draine/scat/bhmie/bhmie.f

MIEV0

The Mie scattering program by W. Wiscombe. For documentation see `libsrc_f/MIEV.doc` and the NCAR Mie report at ftp://climate1.gsfc.nasa.gov/wiscombe/Single_Scatt/Homogen_Sphere/Exact_Mie/

mimcut

(positive) value below which imaginary refractive index is regarded as zero (computation proceeds faster for zero imaginary index). Only used by `mie_program MIEV0`.

```
mimcut value
```

nmom

Number of moments of the phase function to be calculated (default: 0).

```
nmom value
```

Only possible with `mie_program MIEV0`.

nmom_netcdf

Specify the number of Legendre polynomials that are written to the netcdf file.

```
nmom_netcdf value
```

This option only makes sense if `output_user netcdf` is specified. If not specified, all polynomials are written. For the calculation of the phase function all polynomials are of course considered.

numang

Number of angles of the phase function to be calculated (default: 0). For `output_user netcdf` this option is ignored.

```
numang value
```

Currently only implemented for `mie_program` `BHMIE`.

n_r_max

This option makes sense in combination with `distribution GAMMA` or `distribution LOGNORMAL`. It defines the upper cutoff value for the size distribution in terms of effective radius r_{eff}. The default is 5, which means that the size distribution is cut off at a value of $5 \cdot r_{\text{eff}}$. This value should be increased if only small r_{eff} are calculated.

nstokes

Number of Stokes parameters (default: 1).

```
nstokes value
```

For `nstokes=1` the Legendre polynomials of the phase function will be calculated. To calculate all phase matrix elements required for polarized radiative transfer, set `nstokes=4`.

nthetamax

Specify the maximum number of scattering angles to be used to sample the phase matrix.

```
nthetamax value
```

The default value is 1000. If the accuracy of the phase function is less than 1% for `nthetamax` angles a warning is printed to the screen. The option is only meaningful in combination with `output_user netcdf`, otherwise phase functions are not computed.

output_user

The mie output is one line of output quantities to standard output (stdout) for each wavelength and each particle radius. With this option the user may specify the columns desired for output:

```
output_user output_1 output_2 ... output_n
```

where output_i is one of following arguments:

lambda

Wavelength in nm.

wavenumber
Wave number in cm-1.

r_eff
particle radius in micro meter.

refrac_real
The real part of the refractive index.

refrac_imag
The imaginary part of the refractive index.

qext
The extinction efficiency factor, if `r_eff` is specified, or the extinction coefficient [km-1] per unit concentration [cm^3/m^3], if a size distribution (`distribution` or `size_distribution_file`) is specified. If the medium is liquid water, 1 cm^3/m^3 equals a liquid water content of $1g/m^3$ because the density of water is close to 1 g/cm^3. For ice and other substances, the density has to be considered (0.917 g/cm^3 for ice at 273K).

qsca
The scattering efficiency factor, if `r_eff` is specified, or the scattering coefficient [km-1] per unit concentration [cm^3/m^3], if a size distribution (`distribution` or `size_distribution_file`) is specified.

qback
The backscattering efficiency factor, if `r_eff` is specified, or the backscattering coefficient [km-1] per unit concentration [cm^3/m^3], if a size distribution (`distribution` or `size_distribution_file`) is specified. Works only with `mie_program BH`.

omega
The single scattering albedo.

gg
The asymmetry parameter.

sforw
(Complex) forward-scattering amplitude S1 at 0 degrees.

sback
(Complex) back-scattering amplitude S1 at 180 degrees.

spike
To quote from Wiscombe's `MIEV0.doc`:

> (REAL) magnitude of the smallest denominator of either Mie coefficient (a-sub-n or b-sub-n), taken over all terms in the Mie series past N = size parameter XX. Values of SPIKE below about 0.3 signify a ripple spike, since these spikes are produced by abnormally small denominators in the Mie coefficients (normal denominators are of order unity or higher). Defaults to 1.0 when not on a spike. Does not identify all resonances (we are still working on that).

Meaningless if a `size_distribution_file` was specified.

pmom
The nmom+1 moments (from 0 to nmom, see option nmom) of the phase function. The phase function $p(\mu)$ is

$$p(\mu) = \sum_{m=0}^{\infty} (2m+1) \cdot k_m \cdot P_m(\mu) \tag{6.12}$$

where k_m is the m'th moment and $P_m(\mu)$ is the m'th Legendre polynomial.

cloudprp
This is a special option which, if specified, must be the only option of output_user, as cloudprp specifies a whole format of the output. In particular this option is useful when a correlated-k wavelength grid is specified with wavelength. If specified, the output will be written in a format, which can be directly used by *libRadtran*. See also output netcdf. See uvspec-options ic_properties and wc_properties and there the items mie and filename.

aerosolprp
This option is similar to the cloudprp option. The only difference is that the effective radius dimension is replaced by humidity values of the aerosol.

netcdf
This option writes the output to a netCDF file which can be used by uvspec using the options ic_properties and wc_properties.

The default output is:

```
lambda refrac_real refrac_imag qext omega gg spike pmom
```

phase_from_amplitudes
Calculate phase function from scattering amplitudes instead from moments. This option is slower for small size parameters and considerable faster for very large size parameters.

r_eff
The radius [micron] of the particle to calculate single scattering properties of. Used together with the wavelength information to calculate the Mie size parameter.

```
r_eff radius
```

The user can optionally specify a 2nd and 3rd argument to make a loop over several radii:

```
r_eff radius_min radius_max radius_step
```

Alternatively, a logarithmic grid may be defined by specifying a multiplicative increment (indicated by the keyword log):

```
r_eff radius_min radius_max radius_increment log
```

In this case the radius is increased by a factor `radius_increment` for each step.

refrac

Specify which refractive index to use.

```
refrac type
```

The following choices for `type` are valid:

ice

The complex refractive index is taken from the REFICE function by Warren (1984).

water

The complex refractive index is taken either from Segelstein (1981); Warren (1984) or from the more recent IAPWS data set (see `water_properties`)

user

<re> <im> A user defined refractive index. re and im are the real and imaginary parts (both positive numbers).

file

<filename> Read refractive index from a three-column file containing wavelength [nm], and the real and imaginary parts of the refractive index (both positive numbers). The Mie calculation is done for each wavelength defined here.

size_distribution_file

Specify a two column file, r [micron], dn(r)/dr, which describes a size distribution of droplets.

```
size_distribution_file file
```

The Mie calculation is repeated for each value of r found in the size distribution file, and the final result is a weighted average of these values. The user himself has to choose a set of r's suited for his specific purpose.

temperature

Ambient temperature, used to calculate the refractive indices of water and ice.

```
temperature value
```

For Segelstein (1981); Warren (1984) the temperature dependence is only considered above 10 micron (water) and 167 micron (ice), respectively. For IAPWS the temperature dependence is considered for the full wavelength range covered (200 - 1100nm). Default: 300K.

theta_user

User-defined angle grid for netcdf output

```
theta_user theta_min theta_max ntheta
```

Calculate phase function at a user-defined grid instead of providing phase function at an optimized grid.

verbose

If specified abundances of informative messages are output to stderr. To make use of this information, you may want to write the standard mie output to one file and the diagnostic messages to another. To do so, try `(mie < mie.inp > mie.out) >& verbose.txt` (depending on your shell you might need a slightly different syntax).

water_properties

Complex index of refraction either from Segelstein (1981); Warren (1984) or from the more recent IAPWS data set (Wagner and Pruß, 2002).

```
water_properties segelstein/iapws
```

IAPWS only provides the real part of the refractive index. The imaginary is always provided by Segelstein (1981); Warren (1984). For Segelstein (1981); Warren (1984) the temperature dependence is only considered above 10 micron (water) and 167 micron (ice), respectively. For IAPWS the temperature dependence is considered for the full wavelength range covered (200 - 1100nm). Default: 300K.

wavelength

Sets the wavelength range, in nm.

```
wavelength lambda_min lambda_max
```

The wavelength step is specified by `wavelength_step`. For unregular wavelength grid it is also possible to specify a file, where the wavelength grid is stored.

```
wavelength wvl_filename
```

where `wvl_filename` is the path and name of the file, which contains the wavelength grid. It is expected that the wavelength values in nm are stored in the second column. For the `correlated_k` schemes implemented in `uvspec` you can use following abbrevations instead of a filename (in this case `data_files_path` must be specified also): `kato`, `kato2`, `kato2andwandji`, `kato2.96`, `fu`, and `avhrr_kratz`. This option is ignored if `refrac file` is specified.

wavelength_step

The wavelength step, in nm. Ignored if `refrac file` is specified.

```
wavelength_step value
```

wavelength_index

Set the wavelengths to be selected. This might be the normal wavelength grid defined by `wavelength` and `wavelength_step` or a `correlated_k` wavelength grid. E.g., in combination with `wavelength AVHRR_KRATZ`, `wavelength_index 15 15` will select wavelength index 15 which corresponds to channel 4, or `wavelength_index 10 14` will select those bands required for channel 3. Indices start from 1.

write_all_phasefunctions

Write phase functions for all effective radii to a separate netcdf file phase.cdf. Only if `phase_from_amplitudes` is enabled.

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