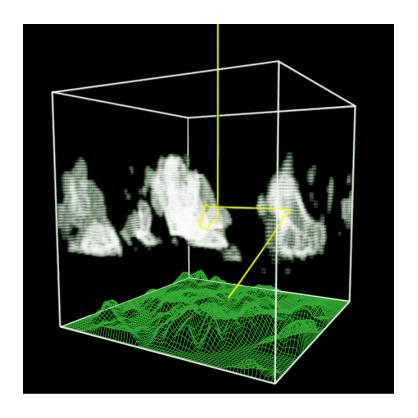
# libRadtran user's guide

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September 21, 2012

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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  $\mu$ m. 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), a fast two-stream code (Kylling et al., 1995), a polarization-dependent code polRadtran (Evans and Stephens, 1991), 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). 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.

2 Preface

## Acknowledgements

Many people have already contributed to *libRadtran*'s development. In addition to Bernhard Mayer (bernhard.mayer (at) dlr.de), Arve Kylling (arve.kylling (at) gmail.com), Claudia Emde (claudia.emde (at) lmu.de), Robert Buras (robert.buras (at) lmu.de), and Ulrich Hamann (ulrich.hamann (at) dlr.de) the following people have contributed to *libRadtran* or helped out in various other ways (the list is almost certainly incomplete – please let us know if we forgot somebody):

- The disort solver was developed by Knut Stamnes, Warren Wiscombe, S.C. Tsay, and K. Jayaweera
- The translation from disort to the cdisort solver was performed by Timothy E. Dowling
- Warren Wiscombe provided the Mie code MIEVO, and the routines to calculate the refractive indices of water and ice, REFWAT and ICEWAT.
- Seiji Kato (kato (at) aerosol.larc.nasa.gov) provided the correlated-k tables described in Kato et al. (1999).
- Tom Charlock (t.p.charlock (at) larc.nasa.gov), Quiang Fu (qfu (at) atm.dal.ca), and Fred Rose (f.g.rose (at) larc.nasa.gov) provided the most recent version of the Fu and Liou code.
- David Kratz (kratz (at) aquila.larc.nasa.gov) provided the routines for the simulation of the AVHRR channels described in Kratz (1995).
- Frank Evans (evans (at) nit.colorado.edu) provided the polradtran solver.
- Ola Engelsen provided data and support for different ozone absorption cross sections.
- Albano Gonzales (aglezf (at) ull.es) included the Yang et al. (2000), Key et al. (2002) ice crystal parameterization.
- Tables for the radiative properties of ice clouds for different particle "habits" were obtained from Jeff Key and Ping Yang, Yang et al. (2000), Key et al. (2002). In addition, Ping Yang and Heli Wei kindly provided a comprehensive database of particle single scattering properties which we used to derive a consistent set of ice cloud optical properties for the spectral range 0.2 100 micron following the detailed description in Key et al. (2002). A comprehensive dataset including the full phase matrices has been generated and provided by Hong Gang.
- Paul Ricchiazzi (paul (at) icess.ucsb.edu) and colleagues allowed us to include the complete gas absorption parameterization of their model SBDART into uvspec.

- Luca Bugliaro (luca.bugliaro (at) dlr.de) wrote the analytical TZS solver (thermal, zero scattering).
- Sina Lohmann (sina.lohmann (at) dlr.de) reduced the "overhead time" for reading the Kato et al. tables dramatically which resulted in a speedup of a factor of 2 in a twostr solar irradiance calculation.
- Detailed ice cloud properties were provided by Bryan Baum (bryan.baum (at) ssec.wisc.edu).
- Yongxiang Hu (yongxiang.hu-1 (at) nasa.gov) provided the delta-fit program used to calculate the Legendre coefficients for ic\_properties baum\_hufit.
- UCAR/Unidata for providing the *netCDF* library.
- Many unnamed users helped to improve the code by identifying or fixing bugs in the code.

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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<sup>1</sup>

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

Here, the photon distribution function  $f(\mathbf{r}, \hat{n}, \nu, t)$  varies with location  $(\mathbf{r})$ , direction of propagation  $(\hat{n})$ , frequency  $(\nu)$  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  $\nu$  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

<sup>&</sup>lt;sup>1</sup>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  $\mathbf{r}$  and  $\mathbf{v}$  are independent variables, Eq. 2.1 may be written as

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

where the  ${\bf r}$  subscript on the gradient operator  $\nabla$  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)

$$\hat{n} \cdot \nabla = n_x \frac{\partial}{\partial x} + n_y \frac{\partial}{\partial y} + n_z \frac{\partial}{\partial z}$$

$$= \cos \phi \sqrt{1 - \mu^2} \frac{\partial}{\partial x} + \sin \phi \sqrt{1 - \mu^2} \frac{\partial}{\partial y} + \mu \frac{\partial}{\partial z}, \tag{2.9}$$

where  $(n_x, n_y, n_z)$  are the components of the unit vector,  $\mu = \cos \theta$  and  $\phi$  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<sup>2</sup>

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

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

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

<sup>&</sup>lt;sup>2</sup>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<sup>3</sup>

$$h\nu \ Q(r,\hat{n},\nu) = h\nu \ Q(r,\theta,\phi,\nu) = -\beta^{ext}(r,\nu) \ I(r,\theta,\phi,\nu)$$

$$+ \frac{1}{4\pi} \int_0^\infty \beta^{sca}(r,\nu,\nu') \int_0^{2\pi} d\phi' \int_0^\pi d\theta' p(r,\theta,\phi;\theta',\phi') I(r,\theta',\phi',\nu') d\nu'$$

$$+ \beta^{abs}(r,\nu) \ B[T(r)]. \tag{2.14}$$

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  $\beta^{emi}$  is equal to the absorption coefficient  $\beta^{abs}$ .

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

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

$$\beta^{abs}(r,\nu) = \sum_{i} \beta_{i}^{abs}(r,\nu), \qquad \beta_{i}^{abs}(r,\nu) = n_{i}(r)\sigma_{i}^{abs}(\nu)$$

$$\beta^{sca}(r,\nu) = \sum_{i} \beta_{i}^{sca}(r,\nu), \qquad \beta_{i}^{sca}(r,\nu) = n_{i}(r)\sigma_{i}^{sca}(\nu)$$
(2.15)

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

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

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

<sup>&</sup>lt;sup>3</sup>For a derivation of the individual terms see e.g. Chandrasekhar (1960).

<sup>&</sup>lt;sup>4</sup>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  $\Theta$  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<sup>5</sup> radiative transfer equation 2.8 is written by combining Eq. 2.10 and Eq. 2.14

$$-\mu \frac{dI(z,\mu,\phi)}{\beta^{ext}dz} = I(z,\mu,\phi)$$

$$-\frac{\omega(z)}{4\pi} \int_{0}^{2\pi} d\phi' \int_{-1}^{1} d\mu' p(z,\mu,\phi;\mu',\phi') I(z,\mu',\phi')$$

$$-(1-\omega(z))B[T(z)]$$
(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  $4 \times 4$  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.

<sup>&</sup>lt;sup>5</sup>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

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

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

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

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 ( $z=z_{\rm toa}$ ) a parallel beam of sunlight with magnitude  $I^0$  in the direction  $\mu_0$  may be present

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

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

where  $\mu_0$  and  $\phi_0$  are the solar zenith and azimuth angles respectively. Inserting Eq. 2.23 into Eq. 2.8 it is seen that the direct beam satisfies

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

$$-\mu \frac{dI(\tau, \mu, \phi)}{d\tau} = I(\tau, \mu, \phi)$$

$$-\frac{\omega(r)}{4\pi} \int_{0}^{2\pi} d\phi' \int_{-1}^{1} d\mu' p(\tau, \mu, \phi; \mu', \phi') I(\tau, \mu', \phi)$$

$$-(1 - \omega(\tau)) B[T(\tau)]$$

$$-\frac{\omega(\tau) I^{0}}{4\pi} p(\tau, \mu, \phi; \mu_{0}, \phi_{0}) e^{-\tau/\mu_{0}}.$$
(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  $\tau/\mu_0$  in Eqs. 2.25 and 2.26 is replaced by the Chapman function,  $ch(r, \mu_0)$  (Rees, 1989; Dahlback and Stamnes, 1991)

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

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

$$-\mu \frac{dI(\tau, \mu, \phi)}{d\tau} = I(\tau, \mu, \phi)$$

$$-\frac{\omega(r)}{4\pi} \int_{0}^{2\pi} d\phi' \int_{-1}^{1} d\mu' p(\tau, \mu, \phi; \mu', \phi') I(\tau, \mu', \phi)$$

$$-(1 - \omega(\tau)) B[T(\tau)]$$

$$-\frac{\omega(\tau) I^{0}}{4\pi} p(\tau, \mu, \phi; \mu_{0}, \phi_{0}) e^{-ch(\tau, \mu_{0})}.$$
(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<sup>6</sup>  $(\mu \ge 0)$ 

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

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

$$I(\tau = \tau_g, \mu, \phi) = \epsilon(\mu) B[T(\tau_g)] + \frac{1}{\pi} \mu_0 I_0 e^{-\tau_g/\mu_0} \rho(\mu, \phi; -\mu', \phi')$$

$$+ \frac{1}{\pi} \int_0^{2\pi} d\phi' \int_0^1 \rho(\mu, \phi; -\mu', \phi') I(\tau, -\mu', \phi') \mu' d\mu', \qquad (2.31)$$

where  $T(\tau_q)$  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

$$\pi I(\tau_L, \mu) = \pi \epsilon B[T(\tau_g)] + \mu_0 A I^0 e^{-\tau_g/\mu_0}$$

$$+2\pi A \int_0^{2\pi} d\phi' \int_0^1 \mu I(\tau_L, -\mu, \phi) d\mu.$$
(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 $\Phi$ -dependence, Fourier decomposition

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

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

<sup>&</sup>lt;sup>6</sup>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

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

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

$$-\mu \frac{dI^{m}(\tau,\mu)}{d\tau} = I^{m}(\tau,\mu)$$

$$-\frac{\omega(r)}{2} \int_{-1}^{1} d\mu' \sum_{l=m}^{2M-1} (2l+1)g_{l}(\tau)\Lambda_{l}^{m}(\mu)\Lambda_{l}^{m}(\mu')I^{m}(\tau,\mu')$$

$$-\delta_{m0}(1-\omega(\tau))B[T(\tau)]$$

$$-\frac{\omega(\tau)I^{0}}{4\pi}(2-\delta_{m0}) \sum_{l=m}^{2M-1} (2l+1)g_{l}(\tau)\Lambda_{l}^{m}(\mu)\Lambda_{l}^{m}(\mu')e^{-\tau/\mu_{0}}.$$
(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

$$I^{\operatorname{dir}}(\tau, \mu_0, \phi_0). \tag{2.40}$$

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

$$E^{+}(\tau) = \int_{0}^{2\pi} d\phi \int_{0}^{1} \mu I(\tau, \mu, \phi) d\mu$$
 (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.

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

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

The various radiative transfer equation solvers included in the uvspec tools in the *libRad-tran* 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))

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

where N(r) is the number of detected photons,  $E_0$  is the energy per laser pulse,  $E_{\rm phot}$  is the energy per photon,  $A_{\rm det}$  is the detector area,  $\eta$  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

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

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

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

where  $r_{\text{surf}}$  is the range of the surface, a is the surface albedo, and  $\theta_{\text{refl}}$  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. 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 file description is

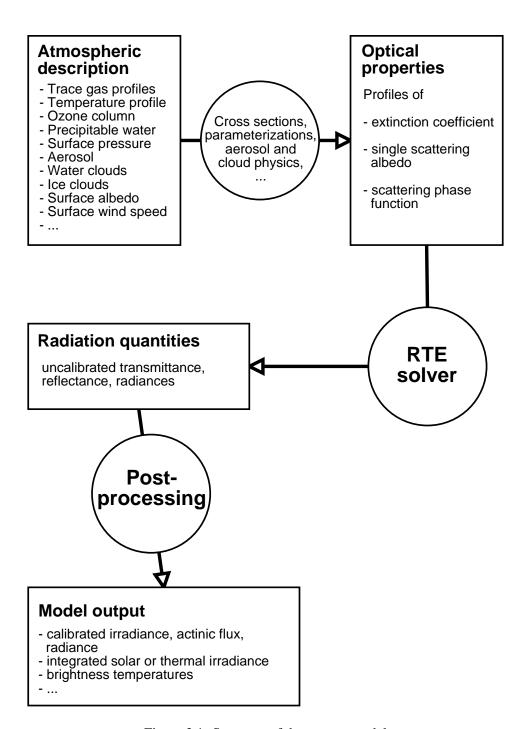


Figure 3.1: Structure of the uvspec model

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followed by several examples of usage of *uvspec*. Finally the radiative transfer equation solvers available in *uvspec* are briefly described.

### 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<sup>1</sup>:

```
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.

<sup>&</sup>lt;sup>1</sup>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

First you need to think about the spectral range and spectral resolution required for your calculation. As long as you stay in the ultraviolet or the lower visible spectral range you don't need to consider anything. Molecular absorption varies smoothly with wavelength in this range and a calculation with 0.5 or 1 nm step width should be sufficient. Above 500nm, however, absorption by water vapour, oxygen, and other trace gases starts; these absorption lines are very narrow, and a spectral calculation which resolves all lines is not feasible for most applications (such a line-by-line calculation is possible, however, if you provide your own spectral absorption cross sections). For most applications you need to select a correlated k-distribution, e.g. correlated\_k lowtran which allows pseudo-spectral calculations (meaning that you still can calculate radiation at any wavelength you want, but the gas absorption is provided only at limited resolution - if you select the wavelengths too close, you will see the steps in your spectrum). For a spectral or pseudo-spectral calculation, you may define your own wavelength grid with transmittance\_wl\_file and we recommend to do that because otherwise you get the default 1nm step which might be too expensive for your application. Finally, in order to calculate integrated shortwave or integrated longwave radiation, please choose one of the pre-defined correlated-k distributions, e.g. correlated\_k kato2 or correlated\_k fu because these are not only much more accurate but also much faster than a pseudospectral calculation. Please read the respective sections in the manual to become familiar with the correlated\_k 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  $3\mu$ m) 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

3.1 BASIC USAGE

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 phi 0. 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 =  $180^{\circ}$  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: afglms (mid-latitude summer), afglmw (mid-latitude winter), afglss (sub-arctic summer), afglsw (sub-arctic winter), afglt (tropical), and afglus (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. ozone\_column which modifies the ozone column, or co2\_mixing\_ratio, âĂę

#### (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\_oric\_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, âĂę - 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

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

and an ic\_file

```
# 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  $10\mu$ m between 1 and 2 km, and an optical thickness of around 15; the second is an ice cloud with

effective particle radius  $20\mu m$  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 cox\_and\_munk\_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 <code>disort2</code> which is the method of choice for most applications. There are other solvers like <code>rte\_solver twostr</code> (faster but less accurate), <code>rte\_solver polradtran</code> (polarization-dependent solver), or <code>rte\_solver sdisort</code> (pseudo-spherical), or <code>rte\_solver mystic</code> (three-dimensional, polarization-dependent solver). Even lidars can be simulated using <code>rte\_solver sslidar</code>.

#### 6. Postprocessing

The spectral grid of the output is defined by the extraterrestrial spectrum. If you want spectrally integrated results, use either correlated\_k kato2 and output sum or correlated\_k lowtran and output integrate. Check also other options like filter\_function\_file, brightness, etc. Instead of calibrated spectral quantities you might also want transmittance or 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 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.

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#### fdisort1, sdisort and spsdisort

For the fdisort1, 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

and so on for each wavelength.

#### twostr, twostrpp, and rodents

The format of the output line for the twostr solver is

```
lambda edir edn eup uavg
```

for each wavelength.

#### polradtran

The output from the polradtran solver depends on the number of Stokes parameters, polradtran\_nstokes.

If phi is not specified the output block is for each wavelength

```
lambda down_flux(1) up_flux(1) ... down_flux(is) up_flux(is)
```

Here is is the number of Stokes parameters specified by polradtran\_nstokes.

If phi and umu are specified the block is

Note that polradtran outputs the total (=direct+diffuse) downward flux. Also note that u0u is always zero for polradtran.

#### 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 3.1.4 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).

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Symbol	Description
cmu	Computational polar angles from polradtran.
down_flux,up_flux	The total (direct+diffuse) downward (down_flux) and up-
	ward (up_flux) irradiances. Same units as extraterrestrial
	irradiance (e.g mW/( $m^2$ nm) if using the atlas3 spectrum
	in the data/solar_flux directory.)
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 ob-
	tain the actinic flux, multiply the mean intensity by $4\pi$ (same
	unit as edir).
uavgdir	Direct beam contribution to the mean intensity (same unit as
	edir).
uavgdn	Diffuse downward radiation contribution to the mean inten-
	sity (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 <sup>2</sup> nm sr) if using the
	atlas3 spectrum in the data/solar_flux directory.)
uu	The radiance (intensity) at umu and phi user specified an-
	gles (unit e.g. $mW/(m^2 \text{ nm sr})$ if using the atlas3 spec-
	trum 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 <sup>2</sup> 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: //climatel.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 (fdisort1, fdisort2, cdisort)

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*.

**fdisort** The original DISORT version 1.3.

fdisort2 The DISORT version 2.0, with several improvements.

**cdisort** The C version of DISORT version 2.0, 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 **disort2** included in *uvspec* further improves the treatment of peaked phase functions.

**cdisort** is the C version of the 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 the modified version 2.0. The default RTE solver in *uvspec* is **cdisort**. If you are worried about spherical effects please use the additional option cdisort pseudospherical.

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

RTE	Geometry	Radiation	Reference	Comments
solver		quantities		
DISORT 1.3	1D, PP	E, F, L	Stamnes et al. (1988)	discrete ordinate
DISORT 2.0	1D, PP	E, F, L	Stamnes et al. (2000)	discrete ordinate
cdisort	1D, PP, PS	E, F, L	Buras et al. (submitted)	discrete ordinate
polradtran	1D, PP	E, F, L	Evans and Stephens (1991)	polarization included
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 ref- erence contains errors (see next section)
sdisort	1D, PS	E, F, L	Dahlback and Stamnes (1991)	pseudo-spherical correction, double precision, customized for airmass calculations
qdisort	1D, PS	E, F, L	Kylling and Stamnes (1992)	based on sdisort, includes extra source term used for Raman scattering
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 scat- tering
sslidar	1D, PP	*		
MYSTIC	3D, SP	E, F, L	Mayer (2009); Emde and Mayer (2007); Emde et al. (2010); Buras and Mayer (2011); Emde et al. (2011)	Monte Carlo <sup>(a)</sup>

<sup>(</sup>a) not included in the free package; available in joint projects

Explanation:	PP, plane-parallel	E, irradiance
	PS, pseudo-spherical	F, actinic flux
	SP, fully spherical	L, radiance
	1D, one-dimensional	L(TOA), radiance at top of atmosphere
	3D, three-dimensional	* sslidar: see section 3.1.4.

Bold face E, F, and F indicate vector quantities.

#### 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 dose 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.

#### **General source term (qdisort)**

The **qdisort** solver is similar to **sdisort** with the addition of a general source term to the right in Eq. 2.29. It is only used when Raman scattering is included the calculation.

#### Two-stream solvers (twostr, twostrpp, 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**.

The **twostrpp** solver is simply **twostr** run in plane-parallel geometry.

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. For more information, you are invited to visit our master course "Advanced Atmospheric Physics", next start in October 2011. The solver was implemented by Robert Buras, hence the name "ROberts' Delta-Eddington Two-Stream".

#### 3.2.2 Polarization (polradtran)

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 calculates the thermal radiance at the top of the atmosphere for a non-scattering atmosphere. In this case, the radiative transfer equation reduces to

$$-\mu \frac{dI(z,\mu,\phi)}{\beta^{ext}dz} = I(z,\mu,\phi) - (1-\omega(z))B[T(z)]$$
(3.1)

where  $I(z,\mu,\phi)=I(z,\mu,\phi,\nu)$  represents the spectral radiance at the wavenumber  $\nu$ ,  $\omega(z)=\omega(z,\nu)$  is the single scattering albedo,  $\beta^{ext}=\beta^{ext}(\nu)$  the exctinction coefficient and  $B[T(z)]=B[T(z),\nu]$  is Planck's function for temperature T. This local problem can be solved by assuming a one-dimensional atmosphere that is split into a number of isothermal layers.

#### 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<sup>2</sup> (default: 1m<sup>2</sup>)

sslidar\_E0 Energy of laser pulse in units of J (default: 0.1J)

**sslidar\_eff** Detector efficiency (default: 0.5)

sslidar\_nranges Number of range bins (default: 100)

**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)

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 due 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 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 some of its output in separate files.

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 (either "escape" radiance if mc\_escape was set, or the sampled radiance)
- 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.

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

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
solar_file ../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 (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 explicitly 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
solar_file ../data/solar_flux/atlas_plus_modtran
dens_column 03 300.
                         # Scale ozone column to 300.0 DU
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; formerly fdisort1
deltam on
                        # delta-M scaling on
nstr 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
```

The atmosphere model, i.e. pressure, temperature, and ozone concentration profiles are read from ../data/atmmod/afglus.dat. The extraterrestrial solar flux is read from the file ../data/solar\_flux/atlas\_plus\_modtran.

A wavelength dependent **surface albedo** may be specified using albedo\_file instead of albedo. Non-Lambertian surface reflectance (BRDF) for vegetation and water may also be defined (please note that these require the use of rte\_solver cdisort. The BRDF of vegetation is specified using rpv\_rho0, rpv\_k, and rpv\_theta, following the definition of Rahman et al. (1993b). Wavelength-dependent BRDF for vegetation can be defined with rpv\_file. The BRDF of water surfaces is parameterized following Cox and Munk (1954a,b) and Nakajima and Tanaka (1983). The respective parameters are the wind speed cox\_and\_munk\_ul0, the pigment concentration cox\_and\_munk\_pcl, and the salinity cox\_and\_munk\_sal. A complete description of these parameters is given in section 6.1.

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**. The essential thing to know is that the internal grid is chosen by *uvspec* itself in a reasonable way, if not explicitly defined in the input file with transmittance\_wl\_file or molecular\_tau\_file. The output grid is completely independent of the internal grid and is entirely defined by the solar\_file. The wavelength grid of all other input data (e.g. albedo, optical properties of aerosols and clouds, etc) is 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; and (2), it should be chosen in a reasonable manner to allow reasonable interpolation (which essentially means, dense enough).

In the ultraviolet/visible, *uvspec* uses an internal grid with a step with 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).

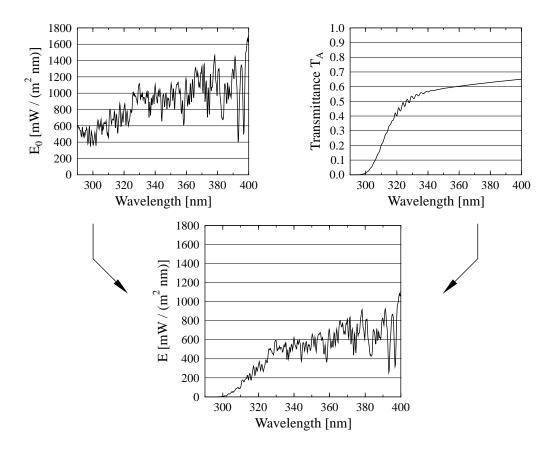


Figure 3.2: *uvspec* calculation of spectral irradiance in the ultraviolet range. (Top left) Low-resolution atmospheric transmittance for US standard atmosphere, solar zenith angle 0°. (Top right) High-resolution extraterrestrial irradiance Kurucz (1992), averaged over 0.1 nm intervals. (Bottom) Product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

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 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 solar\_file which has two important implications: (1) Only those wavelengths are output that are contained in the solar\_file. If e.g. a monochromatic calculation is defined by setting 'wavelength 327.14', there will only be output if the wavelength 327.14 is explicitly listed in 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 solar\_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, solar\_file is a convenient way to define an arbitrary output grid. solar\_file may be omitted for thermal radiation calculations (source thermal) as well as for transmittance and reflectivity calculations. If omitted, the output grid equals the internal wavelength grid.

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If required, a **user-defined internal grid** can be specified with transmittance\_wl\_file or molecular\_tau\_file. 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 one of the correlated\_k parameterizations 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.

#### 3.3.2 Spectral resolution

uvspec offers four 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. **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 and the pseudo-spectral calculation 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 will be the choice for all users interested in the ultraviolet and visible spectral ranges. 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 molecular\_tau\_file. There is no option in libRadtran to generate such a molecular\_tau\_file, 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. genln2 Edwards (1992). Using genln2 it is straightforward to create the input for *uvspec* line-by-line calculations. line-by-line cross sections available for the six standard profiles that come with

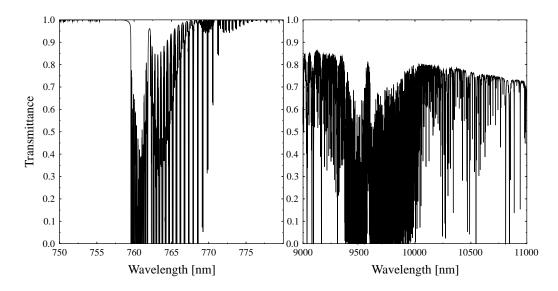


Figure 3.3: Line-by-line calculation of the atmospheric transmittance in two selected solar and thermal spectral ranges, the O2A-absorption band around 760 nm and a region within the infrared window around 10  $\mu$ m.

libRadtran are also available on request. Figure 3.3 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  $10~\mu m$ .

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, and the most accurate of these is the so-called **correlated-k approximation**. *uvspec* contains several correlated-k parameterizations which are invoked with correlated\_k, 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.

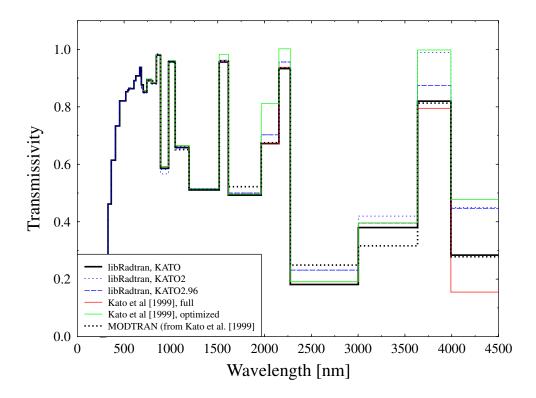


Figure 3.4: Comparison between the three parameterization which are part of *uvspec* and the data from Figure 3 by Kato et al. (1999).

Figure 3.4 shows a comparison between the three parameterization which are part of libRadtran 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 individual 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/(m²nm), but integrated over the spectral bands, e.g. W/m².

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
                         # Correlated-k by Kato et al. [1999]
correlated_k KATO
                         # Calculate integrated solar irradiance
output sum
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 sum to the input file.

For **pseudo-spectral calculations** in the whole spectral range, we have adopted the molecular absorption parameterization from LOWTRAN/SBDART by Ricchiazzi et al. (1998). The respective section of this paper says:

SBDART relies on low-resolution band models developed for the LOW-TRAN 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 <code>correlated\_kLOWTRAN</code>. The spectral resolution may be arbitrarily chosen by the user. If not explicitely defined with <code>transmittance\_wl\_file</code>, 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, <code>data/solar\_flux/kurudz\_l.onm.dat</code> and <code>data/solar\_flux/kurudz\_0.lnm.dat</code>. An example for the solar range is shown in <code>examples/UVSPEC\_LOWTRAN\_SOLAR.INP</code>:

```
atmosphere_file ../data/atmmod/afglus.dat
solar_file ../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
wavelength 250.0 2500.0  # Wavelength range

correlated_k 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
solar_file ../examples/UVSPEC_LOWTRAN_THERMAL.TRANS

source thermal

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

correlated_k LOWTRAN  # select LOWTRAN molecular absorption

output per_nm
quiet
```

Figure 3.5 shows the results of the solar and thermal calculations. The water vapour absorption bands in the solar range are clearly visible, as is the absorption window around 10 micrometer in the thermal. Please note the following points:

• Thermal radiation is per default output in W/(m<sup>2</sup>cm<sup>-1</sup>), if the bandwidth is equal to 1 cm<sup>-1</sup> (default for correlated\_k LOWTRAN calculations). Otherwise the output is the integrated flux over the wavenumber interval specified by

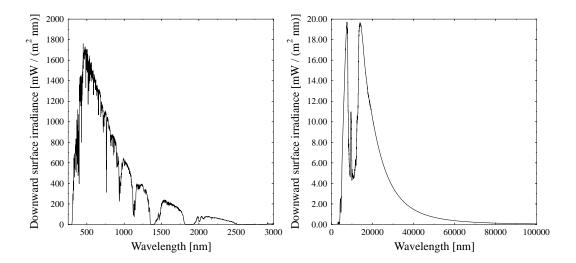


Figure 3.5: Results of the solar and thermal calculations using correlated\_k LOWTRAN.

thermal\_bandwith, thermal\_bands\_file, or by the correlated\_k option (Kato, Kato2, Kato2.96, Fu, AVHRR\_KRATZ, or Generic). To convert e.g. to  $W/(m2\ nm)$  use output per\_nm or multiply with k/lambda where k is the wavenumber [cm $^{-1}$ ] and lambda is the wavelength [nm]. To calculate bandintegrated thermal quantities please consider thermal\_bands\_file.

- Even though no extraterrestrial irradiance is required, a solar\_file may be specified for the thermal case. The reason is that, as explained initially, the solar\_file defines the output grid. The second column in solar\_file can be chosen arbitrarily in this case because it is ignored.
- For the choice of the wavelength grid for the calculation (transmittance\_wl\_grid) 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  $\mu$ m. Choosing higher resolutions for the internal wavelength grid (transmittance\_wl\_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.

Figure 3.6 shows two selected wavelength intervals of the solar and thermal range, to demonstrate the spectral resolution of the LOWTRAN/SBDART absorption parameterization.

The resolution is about 5 cm<sup>-1</sup> 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 both methods.

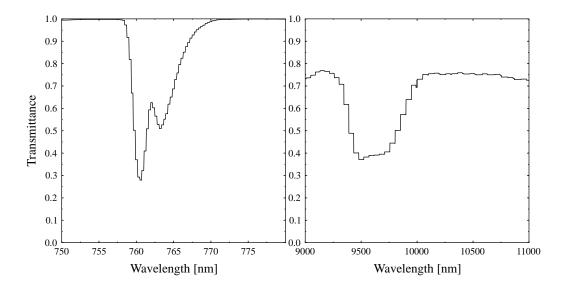


Figure 3.6: Two selected wavelength intervals of the solar and thermal range, to demonstrate the spectral resolution of the LOWTRAN absorption parameterization.

#### 3.3.3 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\_tau\_file, aerosol\_ssa\_file, and aerosol\_qq\_file, 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\_set\_tau or scaled with aerosol\_scale\_tau. The single scattering albedo may be scaled by aerosol\_scale\_ssa or set to a constant value by aerosol\_set\_ssa. The aerosol asymmetry factor may be set by aerosol\_set\_gg. The wavelength dependence of the aerosol optical depth is specified using the aerosol angstrom parameter, aerosol moments file 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 or aerosol\_refrac\_file and the size distribution aerosol\_sizedist\_file. Finally, one may define the aerosol optical properties of each layer explicitely using aerosol\_files.

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 files

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\_tau\_file, aerosol\_ssa\_file, aerosol\_gg\_file

Overwrite profiles of optical thickness, single scattering albedo, and asymmetry parameter

#### aerosol\_moments file

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

#### aerosol\_refrac\_index, aerosol\_refrac file, 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 OPAC aerosol types.

#### aerosol\_set\_gg, aerosol\_set\_ssa, aerosol\_scale\_ssa, aerosol\_set\_tau, aerosol\_scale\_tau

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

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

#### 3.3.4 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 ../examples/WCSIMPLE.DAT # Location of water cloud file
wc_set_tau 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/m3], 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/m3 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/m3 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 wc\_level.

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. 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 correlated\_k kato, correlated\_k 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\_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\_files.

#### 3.3.5 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 tau). Figure 3.7 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  $\mu$ m and from about 3–  $100 \ \mu m$ ). For the calculation of radiances one should use either ic properties baum or ic\_properties hey, because these parameterizations include complete scattering phase functions and do not use approximations like the Heney-Greenstein phase function. ic\_properties hey can also be used for polarized radiative transfer.

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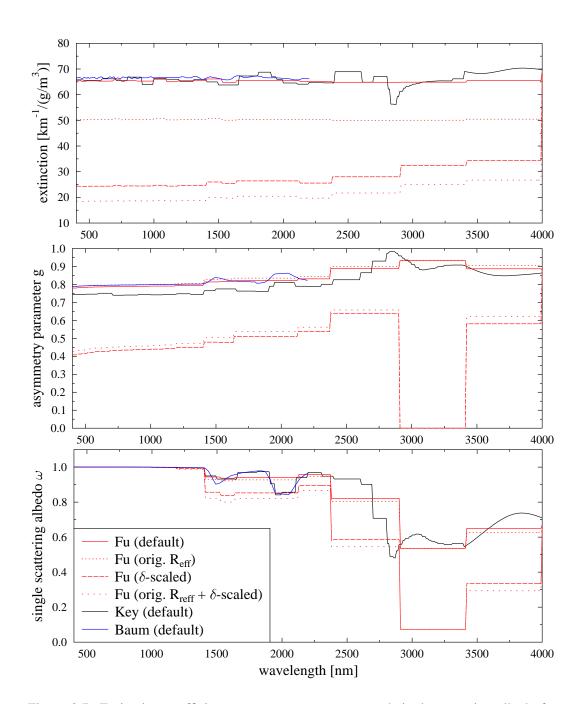


Figure 3.7: Extinction coefficient, asymmetry parameter, and single scattering albedo for ice clouds with an effective radius of 25  $\mu$ m as a function of wavelength for various parameterizations.

#### 3.3.6 Calculation of radiances

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

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:

```
# Location of atmospheric profile file.
atmosphere_file ../examples/UVSPEC_MC_ATM.DAT
                      # Location of the extraterrestrial spectrum
solar_file ../data/solar_flux/atlas_plus_modtran
dens_column 03 300.
                       # Scale ozone column to 300.0 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
mc_photons 100000
                     # 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
```

The keywords here are the same as in input option output\_user.

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 particll with a radius of 200  $\mu$ m. Thew refractive index is specified by the user. The calculation is performed for wavelengths from 200 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
                            # Calculate all phase matrix elements
nstokes 4
nmom 500
                           # Number of Legendre terms to be computed
nmom_netcdf 129
                           # Number of Legendre terms to be stored in
                           #
                               netcdf file, must be > nstr
nthetamax 500
                           # Maximum number of scattering angles to be
                           # used to store the phase matrix
                           # Write output to netcdf file
output_user netcdf
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.

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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 one of the existing standard profiles.

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 <code>Gen\_snow\_tab.pl</code> 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 <code>-help</code> 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 ( $\mu$ m)
- -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 -1 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

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#### 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 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 specified. 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 -1 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
```

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#### 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

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#### -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  $\mu$ .
- -s <step> Step width for evaluation (default: 0.01).
- -o < number of digits > Optimize scattering angle grid.
- -x < filename > File containing  $\mu$ -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).

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-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 -1. 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 <code>Gen\_o3\_tab.pl</code> 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 <code>Gen\_wc\_tab.pl</code> 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 <code>read\_Stamnes\_tab</code> which, for a solar zenith angle and a measured ratio, returns the overhead ozone column or cloud optical depth. The Perl scripts <code>Gen\_o3\_tab.pl</code> and <code>Gen\_wc\_tab.pl</code> 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
```

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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 <code>-lower\_lambda</code> and <code>-upper\_lambda</code>. If absolute units are specified as for filter instruments, use the <code>-absolute</code> 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 <code>Gen\_wc\_tab.pl</code> 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 <code>C program read\_Stamnes\_tab</code> 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)

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

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```
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.

The various input parameters are described in detail below.

### absorption

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

```
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.

# aerosol\_angstrom

Scale the aerosol optical depth using the Ångström formula:

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

where  $\lambda$  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\_files

A way to specify aerosol optical depth, single scattering albedo, and phase function moments for each layer. The file specified by aerosol\_files by

```
aerosol_files file_name
```

has 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 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 cdisort it makes good sense to make the number of moments larger than nstr. For rte\_solver fdisort1 and rte\_solver polradtran the number of moments included in the calculations will be nstr+1. Higher order moments will be ignored for these solvers. Please note that the uppermost line of the aerosol\_files 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\_gg\_file

Location of aerosol asymmetry parameter file specified by

```
aerosol_gg_file file_name
```

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\_files. Comments start with #. Empty lines are ignored.

# 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.
- 2 Maritime type aerosols.
- **5** Urban type aerosols.
- **6** Tropospheric type aerosols.

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

# aerosol moments file

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

```
aerosol_moments_file file_name
```

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

$$p(\mu) = \sum_{m=0}^{\infty} (2m+1) \cdot k_m \cdot P_m(\mu)$$
 (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 <code>aerosol\_set\_gg</code>. The phase function will be the same for all altitudes and wavelengths. See <code>aerosol\_files</code> if more flexibility is wanted. May only be used together with the <code>cdisort</code> or <code>fdisort2</code> solver in combination with the option <code>disort\_icm</code> moments.

### aerosol\_no\_scattering

Switch off scattering by aerosols.

### 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\_refrac\_file

The command line

aerosol\_refrac\_file file\_name

specifies the file containing the wavelength-dependent refractive index of the aerosol. Three columns are expected: wavelength [nm] and the real and imaginary parts of the refractive index. Together with aerosol\_sizedist\_file this forms the input to Mie calculations of the aerosol optical properties. Please note that only the single-scattering albedo, the scattering phase function, and the wavelengthdependence of the extinction coefficient are affected by the Mie calculation while the absolute value of the extinction coefficient is taken from other sources; generally, the extinction coefficient at the first internal wavelength is taken from whatever is available (either default Shettle (1989) or user-defined); the extinction at all other wavelengths is scaled according to the Mie calculation. For this reason, the absolute numbers are not relevant - only the shape of the size distribution matters. In detail: If the aerosol properties are defined using the refractive index and the size distribution, the wavelength dependence of the optical properties is determined by Mie theory. At present there are at least three ways to define the absolute value of the optical thickness: (1) visibility defines the profile at the first *internal* wavelength; for a monochromatic calculation and in correlated-k mode, the first internal wavelength equals the first wavelength output by uvspec; for spectral calculations, the first wavelength might be a little bit smaller than the first wavelength output by uvspec; (2) aerosol\_tau\_file defines the optical thickness profile at the first internal wavelength; or (3) absolute optical thickness and wavelength-dependence are defined by aerosol\_angstrom. It is recommended to avoid this option and rather to calculate the aerosol optical properties externally e.g. with mie and to pass them to uvspec with aerosol\_files.

# aerosol\_refrac\_index

Wavelength-independent refractive index of the aerosol; if wavelength-dependence is required, use <code>aerosol\_refrac\_file</code> instead. Together with <code>aerosol\_sizedist\_file</code> this forms the input to Mie calculations of the aerosol optical properties. Please see the description of <code>aerosol\_refrac\_file</code> to learn how the optical properties are set up. It is recommended to avoid this option and rather to calculate the aerosol optical properties externally e.g. with mie and to pass them to <code>uvspec</code> with <code>aerosol\_files</code>.

# aerosol\_scale\_ssa

Scale the aerosol single scattering albedo for all wavelengths and altitudes with a positive number. If the resulting scaled single scattering albedo is larger than 1 it is set to 1.

aerosol\_scale\_ssa value

# aerosol\_scale\_tau

Scale the aerosol extinction for all wavelengths and altitudes with a positive number.

aerosol\_scale\_tau value

### 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\_gg

Set the aerosol asymmetry parameter for all wavelengths and altitudes to a constant value 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 a aerosol\_files. It doesn't make sense to modify only the first moment of an explicit phase function.

```
aerosol_set_gg value
```

### aerosol set ssa

Set the aerosol single scattering albedo for all wavelengths and altitudes to a constant value between 0.0 and 1.0.

```
aerosol_set_ssa value
```

# aerosol set tau

Set the aerosol optical thickness for all wavelengths and altitudes to a constant value. The optical thickness defined here is the integral from the user-definded altitude to TOA (top of atmosphere).

```
aerosol_set_tau value
```

### aerosol set tau550

Set the aerosol optical thickness at 550nm. Other wavelengths are scaled accordingly. Note that this option requires for technical reasons that the wavelength interval defined by wavelength does contain 550nm. The optical thickness defined here is the integral from the user-definded altitude to TOA (top of atmosphere).

```
aerosol_set_tau550 value
```

# 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\_sizedist\_file

Aerosol size distribution. Two columns are expected: The radius [micrometer] and the particle number. Together with aerosol\_refrac\_index or aerosol refrac file this forms the input to Mie calculations of the aerosol optical properties. Please note that only the single-scattering albedo, the scattering phase function, and the wavelength-dependence of the extinction coefficient are affected by the Mie calculation while the absolute value of the extinction coefficient is taken from other sources; generally, the extinction coefficient at the first internal wavelength is taken from whatever is available (either default Shettle (1989) or user-defined); the extinction at all other wavelengths is scaled according to the Mie calculation. For this reason, the absolute numbers are not relevant - only the shape of the size distribution matters. For details see also the description of aerosol\_refrac\_file. It is recommended to avoid this option and rather to calculate the aerosol optical properties externally e.g. with mie and to pass them to uvspec with aerosol\_files.

# 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, e.g. the OPAC data set provided with libRadtran. The profile file needs to include vertical profiles for each of these species. This file can be either in <code>netCDF</code>-format (automatically recognized filename extension <code>.nc</code> or <code>.cdf</code>) or in ASCII format. The format of the ASCII file is:

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<sup>-1</sup>'; the data are then automatically converted to g/m<sup>3</sup>.

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.

At the libRadtran webpage we provide the OPAC data set (Hess et al., 1998) which can be directly used with uvspec:

```
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
MITR_SPHEROIDS mineral_transported
```

The aspect ratio distribution from (Kandler et al., 2009) is adapted.

# aerosol\_ssa\_file

Location of aerosol single scattering albedo file.

```
aerosol_ssa_file 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\_files. Comments start with #. Empty lines are ignored.

# aerosol\_tau\_file

Location of aerosol optical depth file.

```
aerosol_tau_file 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\_files. Comments start with #. Empty lines are ignored.

# 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 vulcanic aerosols.
- 3 High vulcanic aerosols.
- 4 Extreme vulcanic 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 surface\_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 surface\_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 surface\_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.

# albedo\_map

This option is preliminary and still subject to change (no wavelength dependency yet)! It gives the possibility to specify a wavelength independent albedo with the help of a netCDF file, which is used in combinition with the options latitude, longitude, and time.

```
albedo_map file [variable_name]
```

Here file is the location of the *netCDF* file, The optional argument allows the name of the albedo variable in the *netCDF* file to be specified (the default name is AL). The albedo must be provided as function of latitude and longitude

AL(lat, lon), and may also depend on time AL(time, lat, lon). The latitude, longitude, and time grids must be provided as doubles double lat(lat), double lon(lon), and double time(time). uvspec reads the value at the nearest pixel to the given latitude and longitude. No spatial interpolation or averaging of the values are performed. If a time-dependent albedo is provided, the albedo data nearest to the specified time will be selected (or linear interpolated if time\_interpolate is switched on).

# 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 <code>zout\_interpolate</code>. 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 <code>src\_f/DISORT.MXD</code>).

### altitude map

Specifies an altitude map which is used in combinition with latitude, longitude in order to select the altitude for the simulation. No interpolation is done between the pixels of the map. The format of the call is:

```
altitude_map file [variable_name]
```

where file is the location of the altitude map file. The map is expected to be in *netCDF* format. The file must contain double lat(lat), double lon(lon), and the altitude variable, where variable\_name is the name of the surface el-

evation variable in the <code>netCDF</code> file. The default name is Z. The altitude variable must be <code>altitude(lat, lon)</code>. For format discribtion see also the example map included in <code>libRadtran</code>, <code>data/altitude/ELEVATION\_GTOPO\_10min.cdf</code>. To use this map in <code>uvspec</code>, you may also use <code>altitude\_map GTOPO</code>. This map has a resolution of 10 arc minutes and the unit of the altitude is meter. Please note that this resolution might not ne adequate for your application. If an altitude in the map is below the lowest level of the <code>atmosphere\_file</code>, the atmospheric profiles are extrapolated assuming a constant gradient for temperature and mixing ratios.

### angstrom

Deprecated option. Same as aerosol\_angstrom.

# 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 mc\_wcloud\_file or mc\_icloud\_file.

```
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 traces gases may be set by dens\_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  $\rho$ , can be calulated 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):

```
afglms Midlatitude Summer (midlatitude_summer)
afglmw Midlatitude Winter (midlatitude_winter)
afglss Subarctic Summer (subarctic_summer)
afglsw Subarctic Winter (subarctic_winter)
afglsus U.S. Standard (US-standard)
which may be chosen by for example
```

```
atmosphere_file tropics
```

or by specifying the 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 tsang u10

Wind speed for ocean BPDF (in m/s) at present only available with rte\_solver montecarlo.

```
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 BRDF, a three-parameter BRDF fit for vegetated and non-vegetated surfaces (Wanner et al., 1997).

```
brdf_ambrals iso_value vol_value geo_value
```

Specify iso, vol, and geo. May be combined with montecarlo, cdisort, and fdisort2.

### brightness

Convert radiances / irradiances to equivalent brightness temperatures.

# cdisort\_pseudospherical

Invokes pseudo-spherical geometry in cdisort. Default is plane-parallel.

# cdisort spherical albedo

Calculate spherical albedo using cdisort. When this option is enabled, only the spherical albedo is calculated. The output is enabled by

```
output_user spher_alb
```

# ch4\_mixing\_ratio

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

```
ch4_mixing_ratio value
```

# 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.

## co2 mixing ratio

The mixing ratio of CO2 in ppm.

```
co2_mixing_ratio value
```

The profile is scaled so that the mixing ratio at the user-defined altitude assumes the specified value.

# correlated k

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

```
correlated_k type
```

to choose between the following types of correlated-k schemes:

**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 decrease 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.

**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 SB-DART (Ricchiazzi et al., 1998); please see the section on "Spectral resolution".

**sbdart** Identical to LOWTRAN.

If <code>correlated\_k</code> kato/kato2/kato2.96/fu/avhrr\_kratz is specified, the extraterrestrial flux is taken from internally defined files specific for each parameterization, not from <code>solar\_file</code>. 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 <code>avhrr\_kratz</code> case are included in the <code>uvspec</code> self check which is initiated with <code>make check</code>.

# cox\_and\_munk\_pcl

Pigment concentration for Cox and Munk (1954a,b) ocean BRDF (in mg/m<sup>-3</sup>).

```
cox_and_munk_pcl value
```

At present only available with rte\_solver cdisort, rte\_solver montecarlo and rte\_solver fdisort2. The number of streams (nstr)

is automatically increased to 16 if  $cox_and_munk$  BRDF is switched on, to avoid numerical problems. The default value is  $0.01 \text{ mg/m}^{-3}$ . To switch on Cox and Munk BRDF, specify any of the  $cox_and_munk$  options and define at least  $cox_and_munk_u10$ .

# cox\_and\_munk\_pcl\_map

A possibility to specify pigment concentration (in mg/m3) for the Cox and Munk ocean BRDF with the help of an *netCDF* file, which is used in combinition with options latitude, longitude, and time.

```
cox_and_munk_pcl_map file [variable_name]
```

where file is the location of the *netCDF* file. *libRadtran* reads the value at the nearest pixel to the given latitude and longitude. No spatial interpolation or averaging of the values is done.

The default name of the pigment concentration variable is chlorophyll, but can be changed with the optional argument variable\_name. The pigment concentration must be provided as function of latitude and longitude, chlorophyll(lat, lon), or additionally may also depend on time chlorophyll(time, lat, lon). If a time-dependent pigment concentration is specified, the pigment concentration will be interpolated according to the option time\_interpolate. All grids must be provided in the file as double lat(lat), double lon(lon), and double time(time).

### cox\_and\_munk\_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).

```
cox_and_munk_sal value
```

At present only available with rte\_solver cdisort, rte\_solver montecarlo and rte\_solver fdisort2. The number of streams (nstr) is automatically increased to 16 if cox\_and\_munk BRDF is switched on, to avoid numerical problems. The default value is 34.3. To switch on Cox and Munk BRDF, specify any of the cox\_and\_munk options and define at least cox\_and\_munk\_u10.

# cox\_and\_munk\_sal\_map

Specify ocean salinity (in ppt) for the Cox and Munk (1954a,b) ocean BRDF with the help of an *netCDF* file, which is used in combinition with the options latitude, longitude, and time.

```
cox_and_munk_pcl_map file [variable_name]
```

where file is the location of the *netCDF* file. *libRadtran* reads the value at the nearest pixel to the given latitude and longitude. No spatial interpolation or averaging of the values is done.

The expected name of the pigment concentration variable is per default salinity, but can be changed with the optional argument variable\_name. The pigment concentration must be provided as function of latitude and longitude, salinity(lat, lon), or additionally may also depent on time salinity(time, lat, lon). If a time-dependent salinity is specified, the salinity will be interpolated according to the option time\_interpolate. All grids must be provided as double lat(lat), double lon(lon), and double time(time).

### cox\_and\_munk\_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 cox\_and\_munk\_uphi or is 0 by default.

### cox and munk u10

Wind speed for Cox and Munk (1954a,b) ocean BRDF (in m/s).

```
cox_and_munk_u10 value
```

At present only available with rte\_solver cdisort, rte\_solver montecarlo, and rte\_solver fdisort2. 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. Also, the number of streams (nstr) 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 cox\_and\_munk options and define at least cox\_and\_munk\_u10.

# cox\_and\_munk\_u10\_map

Specify wind speed (in m/s) for the Cox and Munk (1954a,b) ocean BRDF with the help of an *netCDF* file, which is used in combinition with the options latitude, longitude, and time.

```
cox_and_munk_u10_map file
```

where file is the location of the *netCDF* file. *libRadtran* reads the value at the nearest pixel to the given latitude and longitude. No spatial interpolation or averaging of the values is done.

The file must contain the elements of the wind vector U10 and V10. These must be specified as functions of latitude and longitude U10 (lat, lon), V10 (lat, lon), or additionally may also depent on time U10 (time, lat, lon), V10 (time, lat, lon). If the variable time is present in the file, the wind speed will be interpolated according to the option time\_interpolate. All grids must be provided as double lat(lat), double lon(lon), and double time (time).

# cox\_and\_munk\_uphi

Wind direction for Cox and Munk (1954a,b) ocean BRDF.

```
cox_and_munk_uphi value
```

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.)

# crs\_file

May be used to specify cross sections of O3, NO2, BRO, OCLO, HCHO, O4 and SO2 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 NO2, O3, BRO, OCLO, HCHO, O4 or SO2 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<sup>2</sup>)

# $ctwostr\_pseudospherical$

Invokes pseudo-spherical geometry in ctwostr. Default is plane-parallel.

# 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 <code>solar\_file</code>. 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 cdisort and rte\_solver fdisort2 delta-M scaling is hardcoded to be always on.

# dens\_column

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

```
dens_column species column [unit]
```

where species is one of O3, O2, H2O, CO2, NO2, BRO, OCLO, SO2 or HCHO see also dens\_file. The second argument is the total column value, and the optional third argument is the unit, in which the column is given. The unit can be DU (Dobson units) or CM\_2 (molecules/cm²). The default units are DU for O3, and CM\_2 for all other gases. It is possible to have several dens\_column commands in the input file (maximum one per species). The following sets the NO<sub>2</sub> total column to 1.2 DU.

```
dens column NO2 1.2 DU
```

# dens\_file

Specify density profiles (or matrix, see below) of various traces gases to be included in the radiative transfer calculation. The entry of the input file looks like:

```
dens_file gas_species [unit] filename
```

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), and the oxygen dimer (O4). The gas species is identified by their abbrevations given in the parenthesis above. unit is an optional argument to define the unit of the density. The profiles can be given in particles per cm3 (cm<sup>-3</sup>), in particles per m3 (m<sup>-3</sup>), as volume mixing ratio (vmr), as mass mixing ratio (mmr), or as relative humidity (only for water). The default for unit is cm<sup>-3</sup>. 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 dens\_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.

To scale the profile to a total column value use dens\_column.

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 dens\_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 specie. It may however be combined with profiles of other species. A density matrix can only be used in connection with rte solver sdisort!

### disort icm

Intensity correction method for rte\_solver cdisort 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.

# ECMWF\_atmosphere\_file

Reads in combination with the options latitude, longitude, and time (all mandatory) the pressure, temperature, ozone, and water vapour from an ECMWF *netCDF* data file and will combine it with the data given by the atmosphere\_file.

```
ECMWF_atmosphere_file file
```

No spatial interpolation of the values is done. The atmospheric data nearest to the specified time will be selected (or linearly interpolated if time\_interpolate is switched on). Atmospheric profiles, which are not provided by the ECMWF file (O2, CO2, NO2) are taken from the atmosphere\_file. Per default, also the atmosphere above the ECMWF data is taken from the atmosphere\_file. In order to avoid this, please have a look at the option: ECMWF\_levels\_only.

# ECMWF\_levels\_only

The atmosphere considered in the simulation has the same height range as the data in the ECMWF\_atmosphere\_file/radiosonde-file. No further levels are added above those. This option has only an effect in combination with ECMWF\_atmosphere\_file or radiosonde (this option is identical to radiosonde\_levels\_only).

### ECMWF\_ic\_file

Reads in combination with the options latitude, longitude, and time (all

mandatory) the pressure, temperature, and cloud ice water content (CIWC) and cloud cover (CC) from an ECMWF *netCDF* data file.

```
ECMWF_ic_file file
```

No spatial interpolation of the values is done. The data nearest to the specified time will be selected (or linearly interpolated if time\_interpolate is switched on). In order to use the ECMWF data without cloud overlap assumption, use cloud\_overlap off.

### ECMWF ic reff

This option is preliminary and still subject to change! The ECMWF data only contains cloud water content, but no effective radius. With this option, the effective radius can be specified. There are two possibilities: For a fixed effective radius use the keyword fixed and specify the reff in micrometer.

```
ECMWF_ic_reff fixed reff
```

In order to use the parametrisation by cheng Ou and Liou (1995) use the keyword Ou.

```
ECMWF_ic_reff Ou
```

The default option is Ou.

# ECMWF\_ozone\_climatology

The Integrated Forecast System (IFS) of the ECMWF uses a ozone climatology for radiative transfer instead of the ozone simulated by the IFS. If this option is activated the ozone profile of the atmosphere\_file or ECMWF\_atmosphere\_file is replaced by the ozone climatology by Fortuin and Langematz (1995). (If there is also a dens\_file for ozone, it modifies the ozone climatology profile.)

# ECMWF\_wc\_file

Reads in combination with the options latitude, longitude, and time (all mandatory) the pressure, temperature, and cloud liqid water content (CLWC) and cloud cover (CC) from an ECMWF *netCDF* data file.

```
ECMWF_wc_file file
```

No spatial interpolation of the values is done. The data nearest to the specified time will be selected (or linearly interpolated if time\_interpolate is switched on). In order to use the ECMWF data without cloud overlap assumption, use cloud\_overlap off.

# **ECMWF** wind file

Reads in combination with the options latitude, longitude, and time (all mandatory) the wind components U, V, and W from an ECMWF *netCDF* data file.

```
ECMWF_wind_file file
```

The data nearest to the specified time will be selected (or linearly interpolated, if time\_interpolate is switched on).

# emissivity\_map

This option is preliminary and still subject to change (no wavelength dependency yet)! Specify a wavelength independent emissivity with the help of an netCDF file, which is used in combinition with the options latitude, longitude, and time.

```
emissivity_map file [variable_name]
```

where file is the location of the *netCDF* file. With the optional argument variable\_name the name of the emissivity variable in the *netCDF* file can be specified. (By default the expected name is EMIS.) The emissivity must be specified as function of latitude and longitude EMIS(lat, lon), or additionally may also depent on time EMIS(time, lat, lon). All grids must be provided as double lat(lat), double lon(lon), and double time(time). *libRadtran* reads the value at the nearest pixel to the given latitude and longitude. No spatial interpolation or averaging of the values is done. If the variable time is present in the file, the emissivity data nearest to the specified time will be selected (or interpolated if time\_interpolate is switched on).

# f11\_mixing\_ratio

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

```
fll_mixing_ratio value
```

# f12\_mixing\_ratio

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

```
f12_mixing_ratio value
```

# f22\_mixing\_ratio

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

```
f22_mixing_ratio value
```

# filter\_function\_file

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

```
filter_function_file file
```

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 sum or output integrate this option is useful e.g. to calculate weighted irradiances or actinic fluxes or to simulate broadband or satellite observations.

# filter\_function\_normalize

If specified, the integral of the filter function over wavelength is normalized such that output integrate gives radiative properties per wavelength, averaged over the filter function.

### fisot

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 solar\_file.

### flexstor

Deprecated option use output flexstor instead. Provide output in flexstor format. Must not be combined with header. Also, does not currently work when umu and/or phi is specified.

### 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 solar\_file. The units of the fluorescence should obviously be the same as for the solar source in solar\_file. For wavelength dependent fluorescence use fluorescence\_file. The default fluorescence is 0.0. Currently only works with the cdisort 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 cdisort solver. Furthermore. if raman is not set, transmittance\_wl\_file must be specified with the same resolution as the 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 solar\_file.

# h2o\_mixing\_ratio

The mixing ratio of H2O in ppm. Scale the profile so that the mixing ratio at the

user-define altitude assumes the specified value.

```
h2o_mixing_ratio value
```

# h2o\_precip

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).

```
h2o_precip value
```

### header

Include information on some of the input parameters in the output. May not be combined with flexstor. Please note that the information provided is rather incomplete because this option was introduced quite early and was never updated. For a more complete information please use the verbose option.

### ic\_scale\_gg

Scale the ice cloud asymmetry factor for all wavelengths and altitudes with a float between 0.0 and 1.0.

```
ic_scale_gg value
```

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\_tau.

# ic\_scale\_ssa

Scale the ice cloud single scattering albedo for all wavelengths and altitudes with a float between 0.0 and 1.0.

```
ic_scale_ssa value
```

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\_tau.

### ic\_scale\_tau

Scale the water ice optical thickness for all wavelengths and altitudes. with a float between 0.0 and 1000000.0. Also works for 3d clouds.

```
ic_scale_tau value
```

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\_tau.

### ic\_set\_gg

Set the ice cloud asymmetry factor for all wavelengths and altitudes to 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 a ic\_files. It doesn't make sense to modify only the first moment of an explicit phase function.

```
ic_set_gg value
```

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\_tau.

# ic\_set\_ssa

Set the ice cloud single scattering albedo for all wavelengths and altitudes to a value between 0.0 and 1.0.

```
ic_set_ssa value
```

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\_tau.

### ic set tau

Set the total ice cloud optical depth to a constant value for all wavelengths.

```
ic_set_tau value
```

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 ice clouds can be considered constant, e.g. the ultraviolet region. 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\_tau.

# ic\_set\_tau550

Set the ice cloud optical thickness at 550nm. Other wavelengths are scaled accordingly.

```
ic_set_tau550 value
```

The optical thickness defined here is the integral from the surface at the user-defined altitude to TOA (top of atmosphere). Note that this option requires for technical reasons that the wavelength interval defined by wavelength does contain 550nm. 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\_tau.

# ic fu tau

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

```
ic_fu_tau scaled
```

delta-scaling is switched on, with

```
ic_fu_tau unscaled
```

it 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\_set\_tau/tau550/gg/ssa or ic\_scale\_gg/ssa you now get consistent results with all other ice cloud parameterizations.

# 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 sum or output 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\_cd (heating rates are derived from centered differences of the flux (the default method), local (heating rates are derived from the actinic flux), or layer\_fd (heating rates are derived from forward differences of the flux over one layer. Attention: heating\_rate local introduces new levels into the profile which slightly affects the model output. With layer\_fd, the output is not representative for a *level*, but for the *layer* from the z-level of the line in the output file, where it is written, up to next *output level* above!

## ic cloudcover

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

```
ic_cloudcover value
```

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, where the cloud properties are taken from ic\_file, etc. Please note that, if both wc cloudcover and ic cloudcover are set, both must be equal.

This option is ignored, if the option cloud\_fraction\_file is used.

### ic file

### ic file

Location of file defining ice cloud properties.

```
ic_file file
```

The file must contain three columns. Column 1 is the altitude in km, column 2 the ice water content in grams per cubic meter, and column 3 the effective particle radius in micrometer. Empty lines are ignored. Comments start with #. Note that the definition of cloud altitudes in ic\_file 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 an ice cloud is given in examples/IC.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, see ic\_layer and ic\_level. To switch to the old behaviour, use ic\_level. See section 3.3.5 about ice clouds for a realistic example how the contents of the ic\_file are converted to optical properties.

# ic\_files

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

```
ic_files file
```

The file specified by ic\_files 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 level 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 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 single scattering albedo of the layer.

### Column 4-(nmom+4):

The moments of the scattering phase function.

Note that if using rte\_solver cdisort or rte\_solver fdisort2 it makes good sense to make the number of moments larger than nstr because all moments are used in the calculation. For rte\_solver fdisort1 and rte\_solver polradtran the number of moments included in the calculations will be nstr+1. Higher order moments will be ignored for these solvers. Please note that the uppermost line of the ic\_files 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.

# ic\_fu\_reff

If

```
ic_fu_reff fu
```

is specified, the parameterization uses the original definition of the effective radius as specified in Fu (1996); Fu et al. (1998). By default it uses the same definition of the effective radius as the Key et al. (2002), Yang et al. (2000) and Baum et al. (2005a,b) parameterizations; see discussion of ic properties.

### 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, 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, and droxtal; here all habits are available for effective radii from 5 to 90 micrometers in the wavelength region from 0.2 to 5 micrometers.

# ic\_ipa

Independent column calculation for a 3D cloud field.

```
ic_ipa file
```

As argument a name of a 3D cloud file must be given. This file has to be in the format as needed by MYSTIC, see mc\_wcloud\_file.

### ic ipa files

A two-column file, defining ice cloud property files (see ic\_file) in the first column and the correspoding weights in the second column.

```
ic_ipa_files file
```

The radiative transfer calculation is performed independently for each cloud column and the result is the weighted average of all independent columns. If ic\_ipa\_files and wc\_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.

# ic\_layer

Interpret ice cloud properties as layer properties (this is the default behaviour since version 1.4; see also ic\_file). Cloud properties are assumed to be constant within each layer. The layer reaches from the level where the properties are defined in the ic\_file to the level above that one. For example, the following lines

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

# ic level

Interpret cloud properties as level properties (this was the default behaviour before version 1.4; see also ic\_file). If ic\_level is defined, a ic\_file would be interpreted as follows:

#	Z	IWC	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/m³ 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.

# ic\_no\_scattering

Switch off scattering by ice clouds.

# ic\_properties

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

```
ic_properties type
```

# Possible choices for type 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\_tau scaled 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\_tau and ic\_fu\_reff. 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 habits: solid-column, hollow-column, 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 cdisort, montecarlo, and fdisort2, accurate phase functions are used.

baum\_hufit Similar to the option baum but here the phase function is parameterized by 128 Legendre coefficients, calculated with the delta-fit method from Hu and Stamnes (2000). This parameterization covers the region from 0.4 to 2.2 micrometer. If high accuracy is needed e.g. in the vicinity of the halo, the forward peak, or the backscatter peak, ic\_properties baum is recommended.

hey Use pre-calculated ice cloud optical properties including full phase matrices. This option has newly been implemented and is not yet well validated. Please check your results carefully!! 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

$$n(r) = n_0 r^{\alpha} \exp\left(-\frac{(\alpha+3)r}{r_e}\right),\tag{6.3}$$

where  $n_0$  is found by normalization and  $\alpha$  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 available for the following habits: solid-column, hollow-column, rough-aggregate, rosette-6, plate, and droxtal. The default habit is solid-column. The habit can be specified using the option ic\_habit.

mie Use pre-calculated Mie tables; useful for correlated\_k; the tables are expected in data\_files\_path/correlated\_k/.../. For spectral or pseudo-spectral calculations ic\_properties\_interpolate has to be defined explicitely to initiate the interpolation of the optical properties to the internal wavelength grid. Note that a Mie calculation assumes spherical ice particles, the scattering function of which differs systematically from non-spherical particles. Hence, ic\_properties mie is usually not representative of natural ice clouds.

**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), citeKey2002, and Baum et al. (2005a,b) use the general definition

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

$$\tag{6.4}$$

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

$$r_{\text{eff}} = \frac{\int D^2 L n(L) dL}{2 \int (DL + \frac{\sqrt{3}}{4} D^2) n(L) dL}$$
(6.5)

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 fu 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 fu!

# ic\_properties\_interpolate

Interpolate ice cloud optical properties 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).

# ic saturate

Obsolete option.

### include

Include a file into the uvspec input.

```
include file
```

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

# 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 deg [min] [sec]
```

where deg min sec is the position in degrees, arc minutes, and arc seconds north. 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, time, and any map-option is used to select the location where to read the input data.

latitude in combination with longitude and time is used to calculate the solar zenith angle, if no sza is specified (see also time\_interval).

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 deg [min] [sec]
```

where deg min sec is the position in degrees, arc minutes, and arc seconds east. deg might also be a float number. min and sec may be obmitted. The longitude information will be used for the following:

longitude in combination with latitude, time, and any map-option is used to select the location where to read the input data.

longitude in combination with latitude and time is used to calculate the solar zenith angle, if no sza is specified (see also time\_interval).

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

### 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 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

f 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 basename

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

mc\_basename basename

# mc\_delta\_scaling

Truncate phase function in MYSTIC: The phasefunctions are set to zero for mu>mucut. The extinction coefficient etc. are scaled accordingly. Optional settings are mc\_delta\_scaling mucut and mc\_delta\_scaling mucut n\_start, where mucut is 0.99 by default. The value n\_start defines after which scattering order delta-scaling is applied, before that scattering order, the real phase function is applied. Default is 0, i.e. the delta-scaled phase function is applied from the beginning.

# 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\_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 correlated\_k.

### 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.

### mc refraction

Enable refraction for rte\_solver montecarlo. Works only in 1D spherical geometry (with option mc\_spherical).

# mc\_spherical

Spherical geometry in MYSTIC. Works only in "1D" - wcloud\_file and icloud\_file are not yet considered. If mc\_spherical is selected mc\_backward is switched on automatically.

### 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).

# molecular\_tau\_file

Location of molecular absorption optical depth file.

```
molecular_tau_file file
```

Usually, molecular absorption is calculated from trace gas concentrations provided in atmosphere\_file (scaled with ozone\_column, 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 molecular\_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 transmittance\_wl\_file. molecular\_tau\_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.02A.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.

# n2o\_mixing\_ratio

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

```
n2o_mixing_ratio value
```

# no2\_column\_du

Obsolete, use dens\_column instead.

# no2\_column\_moleccm-2

Obsolete, use dens\_column instead.

### no2 crs

Choose between the various no2 cross sections by

```
no2_crs type
```

where type is one of

# **Burrows**

Burrows et al. (1998) no2 cross section.

# **Bogumil**

no2 cross section from Bogumil et al. (2003).

Bogumil et al. (2003) is default.

# no\_absorption

Switch all (molecular, aerosol, cloud, and ice cloud) absorption off. Please note that this option simply sets the absorption optical thickness to 0. If used together with xxx\_set\_tau this might be a bit confusing but probably the most logical way. E.g. when using aerosol\_default and aerosol\_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.

# $no\_molecular\_absorption$

Switch off molecular absorption.

### no\_rayleigh

Switch Rayleigh scattering off.

## no\_scattering

Switch scattering off.

### nrefrac

For the rte\_solver sdisort refraction may be included by

```
nrefrac value
```

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.

#### nscat

The order of scattering for the sos radiative transfer equation solver.

```
nscat value
```

Default is 20. May also be used with the sdisort solver. If set to 1 sdisort will run in single scattering mode while if set in to 2, sdisort runs in full multiple scattering mode.

### nstr

Number of streams used to solve the radiative transfer equation.

```
nstr value
```

Default is 6 for fluxes and 16 for radiances. (For rte\_solver fdisort1, fdisort2 and cdisort only even nstr are possible.)

### o2\_mixing\_ratio

The mixing ratio of O2 in ppm.

```
o2_mixing_ratio value
```

Scale the profile so that the mixing ratio at the user-defined altitude assumes the specified value.

### o3\_crs

Choose between the various ozone cross sections by

```
o3_crs type
```

where type is one of

### Bass\_and\_Paur

Bass and Paur (1985) ozone cross section.

#### Molina

Molina and Molina (1986) ozone cross section.

#### **Daumont**

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

### **Bogumil**

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

Molina and Molina (1986) is default.

### optimize\_fortran

When this option is activated, the minimum dimensions of the FORTRAN arrays for the specific input conditions are determined and written to stderr. Using worldloop two tolerance levels are added to the minimum number of atmospheric levels, as this number may change during worldloop calculations.

# output

Decide how the output from uvspec is processed:

```
output type
```

where type is one of

#### sum

Sum output over wavelength. Useful in combination with the correlated\_k option (kato, kato2, kato2.96, Fu, avhrr\_kratz).

## integrate

Integrate output over wavelength for solar and over wavenumber for thermal simulations. Useful for spectral calculations and correlated\_k lowtran.

### per\_nm

Output is given in W/(m<sup>2</sup> nm) or mW/(m<sup>2</sup> nm) (W or mW is determined by the extraterrestrial spectrum.)

# $per\_cm^{-1}$

Output is given in  $W/(m^2 \text{ cm}^{-1})$  or  $mW/(m^2 \text{ cm}^{-1})$ .

### per ck band

Output is given in W/m<sup>2</sup> or mW/m<sup>2</sup> per correlated-k band. (This option can not be used for spectral calculations and correlated\_k LOWTRAN in the solar range.)

### none

No processing - output spectral information (default).

# 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\_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 /  $4\pi$ ).

### 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:
     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<sup>-3</sup>]
rho_xxx
     mass density of the gas xxx [kg/m<sup>3</sup>]
mmr_xxx
     mass mixing ratio of the gas xxx [kg/kg]
vmr_xxx
     volume mixing ratio of the gas xxx [m<sup>3</sup>/m<sup>3</sup>]
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<sup>3</sup>]
CIWC
     cloud ice water content [kg/kg]
CIWD
     cloud ice water density [g/m<sup>3</sup>]
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 and the output of rte\_solver polradtran are not affected.

### ozone column

Obsolete, use dens\_column 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.

### polradtran\_aziorder

Order of Fourier azimuth series

```
polradtran_aziorder value
```

The value 0 (default for irradiance) is the azimuthally symmetric case. For radiance computation a higher order is required, thus the default for radiances is 4. This option is only relevant for rte\_solver polradtran.

## polradtran\_max\_delta\_tau

Initial layer thickness for doubling; governs accuracy, 10E-5 should be adequate. Do not go beyond half the real precision, i.e. 10e-8 for REAL\*8. Default 1.e-05.

```
polradtran_max_delta_tau value
```

This option is only relevant for rte\_solver polradtran.

# polradtran\_nstokes

Number of Stokes parameters

```
polradtran_nstokes value
```

where value is one of

- 1 for I (no polarization, default)
- **2** for I,Q,U (Since V is very small in the atmosphere, it makes sense to compute only I,Q,U. This saves computation time and memory).
- 3 for I,Q,U,V

Default is 1.

## polradtran\_quad\_type

Type of quadrature used:

```
polradtran_quad_type type
```

where type is one of

- G gaussian
- D double gaussian,
- L Lobatto
- E (default) extra-angle(s), this must be used of polradtran is used in combination with umu. Will internally use Gaussian scheme (G). See also radtran documentation (libsrc\_f/README.polRadtran).

Default E. This option is only relevant for rte\_solver polradtran.

### polradtran\_src\_code

Radiation sources included by

```
polradtran_src_code value
```

which may be

- 0 none
- 1 solar
- 2 thermal
- 3 both

Default 1. This option is only relevant for rte\_solver polradtran.

### 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.

### prndis

Specify one or more integers between 1 and 7.

```
prndis 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, ic\_file, wc\_files, etc.

Usage:

```
profile_file typename type file
```

typename describes the name of the profile; typically this is describes what kind of particles are dealt with here. Examples are "wc", "ice\_clouds", "aer", "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 can be one of the following (described for the example of water clouds):

- **1d** Location of file defining one-dimensional profile. See wc\_file for a description on the file structure.
- ipa\_files A two-column file, defining one-dimensional profile files (see type 1d)
   in the first column and the corresponding weights in the second column.
   See wc\_ipa\_files for a more thorough description.
- **moments** A way to specify extinction coefficient, single scattering albedo, and scattering phase function for each layer. See wc\_files for a description of the file format.

## profile\_layer

Interpret properties of profile typename as layer properties. (default). See wc\_layer for more explanations.

Usage:

```
profile_layer typename
```

# profile\_level

Interpret properties of profile typename as level properties. See  $wc\_level$  for more explanations.

Usage:

```
profile_level typename
```

### profile\_no\_scattering

Switch off scattering on profile typename. Usage:

```
profile_no_scattering typename
```

### 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
```

typename describes the name of the profile; it must be identical to the one defined in profile\_file.

Possible choices for property are

#### hu

Parameterization by Hu and Stamnes (1993) for water clouds; this is the default setting. Note that the parameterization is somewhat different for correlated\_k 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.

This type is only available for name "wc" and "ic". Dependent on which name is defined, the appropriate parameterization is chosen.

#### mie

Use pre-calculated Mie tables for water and ice clouds; useful for correlated\_k; the tables expected are data\_files\_path/correlated\_k/.../.

For spectral or pseudo-spectral (correlated\_k sbdart) calculations, a set of pre-calculated tables is also available. For spectral or pseudo-spectral calculations wc\_properties\_interpolate has to be defined explicitly 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).

This type is only available for name "wc" and "ic". Dependent on which name is defined, the appropriate parameterization is chosen.

Note that a Mie calculation assumes spherical ice particles, the scattering function of which differs systematically from non-spherical particles. Hence, ic\_properties mie is usually not representative of natural ice clouds.

# filename

Read optical properties from specified filename; file format is as produced by the mie-tool of the *libRadtran* package (see output\_user netcdf).

**fu** Parameterization by Fu (1996); Fu et al. (1998) for ice particles, 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\_tau scaled 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\_tau and ic\_fu\_reff. The allowed range for the effective radius is from 9.315 - 65.120 micrometer.

- **key** Parameterization by Key et al. (2002) for ice particles. 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 habits: solid-column, hollow-column, aggregate, rosette-4, rosette-6, and plate.
- yang Parameterization similar to Key et al. (2002) for ice particles 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 cdisort, montecarlo, and fdisort2, accurate phase functions are used.
- baum\_hufit Similar to the option baum but here the phase function is parameterized by 128 Legendre coefficients, calculated with the delta-fit method from Hu and Stamnes (2000). This parameterization covers the region from 0.4 to 2.2 mi-

crometer. If high accuracy is needed e.g. in the vicinity of the halo, the forward peak, or the backscatter peak, ic properties baum is recommended.

hey Use pre-calculated ice cloud optical properties including full phase matrices. This option has newly been implemented and is not yet well validated. Please check your results carefully!! 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

$$n(r) = n_0 r^{\alpha} \exp\left(-\frac{(\alpha+3)r}{r_e}\right),\tag{6.6}$$

where  $n_0$  is found by normalization and  $\alpha$  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 available for the following habits: solid-column, hollow-column, rough-aggregate, rosette-6, plate, and droxtal. The default habit is solid-column. The habit can be specified using the option ic\_habit.

The default property is hu in case of name "wc" and fu in case of name "wc" and fu. Else the property needs to be specified!

A note on ice particles:

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), citeKey2002, and Baum et al. (2005a,b) use the general definition

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

$$\tag{6.7}$$

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

$$r_{\text{eff}} = \frac{\int D^2 L n(L) dL}{2 \int (DL + \frac{\sqrt{3}}{4} D^2) n(L) dL}$$
(6.8)

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

fu 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 fu!

## profile\_properties\_interpolate

Interpolate optical properties for profile typename over wavelength; useful for precalculated optical property files defined with profile\_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).

```
profile_properties_interpolate typename
```

### profile scale gg

Scale the asymmetry factor of profile typename for all wavelengths and altitudes with a float between 0.0 and 1.0.

```
profile_scale_gg typename value
```

See  $wc\_scale\_gg$  for more explanations.

## profile\_scale\_ssa

Scale the single scattering albedo of profile typename for all wavelengths and altitudes with a float between 0.0 and 1.0.

```
profile_scale_ssa typename value
```

See wc\_scale\_ssa for more explanations.

# profile\_set\_gg

Set the asymmetry factor of profile typename for all wavelengths and altitudes to a float between -1.0 and 1.0.

```
profile_set_gg typename value
```

See wc\_set\_gg for more explanations.

### profile\_set\_ssa

Set the single scattering albedo of profile typename for all wavelengths and altitudes to a float between 0.0 and 1.0.

```
profile_set_ssa typename value
```

See wc\_set\_ssa for more explanations.

### profile\_set\_tau

Set the total optical thickness of profile typename to a constant value for all wavelengths.

```
profile_set_tau typename value
```

See wc\_set\_tau for more explanations.

## profile\_set\_tau550

Set the water optical thickness of profile typename at 550nm.

```
profile_set_tau550 typename value
```

See wc\_set\_tau550 for more explanations.

### 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 cm³ (CM-3), in particles per m³ (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<sup>-3</sup> (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

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 cdisort 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.

Please note that while the raman option has been extensively tested and verified, it is nevertheless a new option, hence, use it with care.

### raman\_original

Treats each wavelength individually and is thus accurate, but computationally very expensive.

### rayleigh\_crs

Specify the Rayleigh cross section.

```
rayleigh_crs type
```

Choose between the following Rayleigh scattering cross sections.

### **Bodhaine**

Bodhaine et al. (1999) Rayleigh scattering cross section.

# Nicolet

Nicolet (1984) Rayleigh scattering cross section.

### **Penndorf**

Penndorf (1957) Rayleigh scattering cross section.

Bodhaine et al. (1999) is default.

### 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 + depol)/(2 + depol) and b = 1.5(1 - depol)/(2 + depol). By default the depolarization is calculated using the expressions from Bodhaine et al. (1999).

## rayleigh\_tau\_file

Location of Rayleigh scattering optical depth file.

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. The format is exactly the same as for molecular\_tau\_file.

### reflectivity

Calculate transmission / reflectivity instead of absolute quantities. For irradiances / actinic fluxes the transmission T is defined as

$$T = \frac{E}{E_0 \cos \theta} \tag{6.9}$$

where E is the irradiance / actinic flux,  $E_0$  is the extraterrestrial flux, and  $\theta$  is the solar zenith angle. The reflectivity R is defined as

$$R = \frac{\pi \cdot L}{E_0 \cos \theta} \tag{6.10}$$

where L is the radiance,  $E_0$  is the extraterrestrial flux, and  $\theta$  is the solar zenith angle. Obviously, reflectivities do not depend on Sun-Earth distance. Please note the difference to transmittance.

#### reverse

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.

### rh\_file

File that defines a profile of relative humidity.

If specified, the water vapour profile in atmosphere\_file is over-written. If -1 is specified at a level, the value from atmosphere\_file is used.

### rpv\_file

4 column file, containing the Rahman, Pinty, and Verstraete (RPV) BDRF parameterization (Rahman et al., 1993a).

```
rpv_file file
```

Bidirectional reflectance distribution functions for a variety of surfaces are given in the paper. This option is only supported with solvers: cdisort, fdisort2 and rte\_solver montecarlo (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.

# rpv\_k

Constant RPV k, see rpv\_file.

```
rpv_k value
```

rpv\_k overwrites the wavelength-dependent value defined in rpv\_file.

### rpv\_library

The rpv libraries are collections of spectral BRDFs of different surface types, This option must be used either with surface\_type or surface\_type\_map, in order to select the specific surface type.

For using a rpv\_library write

```
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 surface\_type 1 is specified the BRDF from IGBP.01.rpv will be used, and so on. Each file must have the structure like an rpv\_file. (This option is quite the same as rpv\_file, except that it offers you an easy way to use the option surface\_type\_map in combinition with your rpv\_files.)

```
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.

### rpv\_rho0

Constant RPV rho0, see rpv file.

rpv0 value

rpv\_rho0 overwrites the wavelength-dependent value defined in rpv\_file.

### rpv\_scale

Apply a constant scaling factor for the RPV BRDF.

```
rpv_scale value
```

Required e.g. if the the albedo should be set to a certain value. This factor is only used by rte\_solver cdisort, rte\_solver fdisort2 and rte\_solver montecarlo.

# rpv\_sigma

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

```
rpv_sigma value
```

A wavelength dependent sigma is not yet available.

### rpv\_t1

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

```
rpv_t1 value
```

A wavelength dependent sigma is not yet available.

### rpv\_t2

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

```
rpv_t2 value
```

A wavelength dependent sigma is not yet available.

### rpv\_theta

Constant RPV theta, see rpv\_file.

```
rpv_theta value
```

rpv\_theta overwrites the wavelength-dependent value defined in rpv\_file.

### rte\_solver

Set the radiative transfer equation solver to be used.

```
rte_solver type
```

If not specified the default rte\_solver is cdisort. Choices for type are

## cdisort

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\_icm moments (like in the original code), or with the improvements described in (Buras, Dowling, Emde, in preparation; default). Can be run in plane-parallel geometry (default) or in pseudo-spherical geometry (using cdisort\_pseudospherical).

#### ctwostr

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 ctwostr\_pseudospherical).

#### disort

Same as cdisort which is the recommended discrete ordinate code in *libRad-tran*. Before *libRadtran* 1.6 cdisort invoked the Fortran code disort 1.3.

#### disort2

Same as cdisort which is the recommended *discrete ordinate code* in *libRad-tran*. Before *libRadtran* 1.6 cdisort invoked the Fortran code disort 2.0.

#### 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://climatel.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 disort2, you need to specify disort\_icm 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 recompile.

### 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.

### polradtran

The plane-parallel radiative transfer solver of Evans and Stephens (1991). Includes polarization. The full implementation of the polRadtran solver in uvspec is quite new (version 1.4). If you find unusual behaviour, please contact the *libRadtran* authors.

#### twostr

The two-stream radiative transfer solver described by Kylling et al. (1995), in pseudo-spherical geometry.

#### twostrpp

The two-stream radiative transfer solver described by Kylling et al. (1995), in plane-parallel geometry.

#### rodents

Delta-Eddington two-stream code (RObert's Delta-Eddington Two-Stream), plane-parallel.

#### 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 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.

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: cdisort

### satellite\_geometry

With this option the satellite geometry is determinded. The argument for this option

```
satellite_geometry netCDF_file
```

is the location of a netCDF\_file, which must contain latitude and longitude position as well as zenith and azimuth viewing angle for each pixel.

## satellite\_pixel

This option specifies which pixel of the satellite image that should be simulated.

```
satellite_pixel pixel_x pixel_y
```

The arguments pixel\_nr\_x and pixel\_nr\_y specifies the pixel position in the native system of the satellite, which is determinded by the option satellite\_geometry.

### 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.

#### solar file

Location of file holding the extraterrestrial spectrum.

```
solar_file filename [unit]
```

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. solar\_file may be omitted for thermal radiation calculations (source thermal) as well as transmittance and 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 purpuses it is useful to tell libRadtran the units of the spectrum. This can be done with the optional second argument. 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). Note that solar\_file is ignored if correlated\_k is specified.

#### 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) for spectral and correlated\_k LOWTRAN calculations. For all other correlated\_k options the output is integrated over the wavelength band. Thermal radiation is per default output in W/(m2 cm-1), if the bandwidth is equal to 1 cm-1 (default for correlated\_k LOWTRAN calculations). Otherwise the output is the integrated flux over the wavenumber interval specified by thermal\_bandwith, thermal\_bands\_file, or by the correlated\_k option (kato, kato2, kato2, 96, fu, or avhrr\_kratz).

## 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\_area

Set area of single scattering lidar in units of square meters (solver sslidar).

# sslidar\_E0

Set Laser pulse energy for single scattering lidar in units of Joule (solver sslidar). (You can also use a solar\_file instead... not yet implemented.)

### sslidar eff

Set lidar efficiency for single scattering lidar (solver sslidar).

# sslidar\_nranges

Set number of range bins for single scattering lidar (solver sslidar).

### sslidar\_polarisation

Turn on polarisation measurement for lidar (solver sslidar).

## sslidar\_position

Set lidar position for single scattering lidar in units of km (solver sslidar).

### sslidar\_range

Set lidar range bin width for single scattering lidar in units of km (solver sslidar).

# surface\_temperature

Surface temperature, used for thermal infrared calculations.

```
surface_temperature value
```

If not specified, the temperature of the lowest atmospheric level is used as surface temperature.

### surface\_temperature\_map

Specify a surface\_temperature map with a *netCDF* file which is used in combinition with the options latitude, longitude, and time.

```
surface_temperature_map file [variable_name]
```

where file is the location of the *netCDF* file. libRadtran reads the value at the nearest pixel to the given latitude and longitude. No spatial interpolation or averaging of the values is done.

# surface\_type

With this option the surface\_type is selected. This option can be used with albedo\_library in order to select a spectral albedo or with rpv\_library in

order to select a BRDF function.

```
surface_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.

### 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 surface\_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 <code>surface\_type\_map</code> <code>IGBP</code>. This map has a resolution of 10 minutes and contains the surface types 1 to 18 defined in the <code>albedo\_library</code> <code>IGBP</code>. 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 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 correlated\_k 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.

## time\_interpolate

If a map option is used in combination with time, the data, which is nearest to the

specified time is used for the simulation. This means time\_interpolate is switched off per default.

If this option is switched on, the data fields stored in the *netCDF* files are interpolated to the specified time. (Be aware, that this might cause strange effects for data field of moving properties. E.g. an interpolated cloud field might have double horizontal extent, but only half the optical depth.)

## time\_interval

This option can be used in order to calculate an effective solar zenith angle for a time interval, instead of a distinct point in time. The cosine of the solar zenith angle is here replaced by its time average. The azimuth of the sun is replaced by an average of the azimuth position weighted with the cosine of the solar zenith angle.

```
time_interval dtime_start dtime_end [unit] time_interval -180 180 min
```

the time interval reaches from time + dtime\_start to time + dtime\_end, in the example from 180 minutes before time to 180 minutes after time. The unit argument is optional, and can be one of the following: s (seconds), min (minutes), or h (hour). The default is s. This option makes only an effect in combination with time, latitude, longitude, and only has an effect for solar simulations (and of course if no sza defined).

#### transmittance

Calculate transmittance / reflectance instead of absolute quantities. That is, set the extraterrestrial irradiance to 1 and do not correct for Sun-Earth distance:

$$T = \frac{E}{E_0} \tag{6.11}$$

where E is the irradiance / actinic flux / radiance and  $E_0$  is the extraterrestrial flux. Please note the difference to reflectivity.

### transmittance\_wl\_file

Location of single column file that sets the wavelength grid used for the internal transmittance calculations.

```
transmittance_wl__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.

#### umu

Cosine of output polar angles in increasing order, starting with negative (down-welling 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 solar\_file, unless spline is specified. Note that the radiative transfer calculations are done on an internal grid which can be influenced with transmittance\_wl\_file or molecular\_tau\_file

### wavelength\_index

Set the wavelengths to be selected. To be used together with predefined wavelength grids, such as transmittance\_wl\_file, molecular\_tau\_file and particularly useful in combination with the correlated\_k option where often only a specified number of wavelength bands is required. E.g., in combination with correlated\_k 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\_cloudcover

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

```
wc_cloudcover value
```

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, where the cloud properties are taken from wc\_file, etc. Please note that, if both wc\_cloudcover and ic\_cloudcover are set, both must be equal.

This option is ignored, if the option cloud\_fraction\_file is used.

## wc file

Location of file defining water cloud properties.

```
wc_file file
```

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 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 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, see wc\_layer and wc\_level. To switch to the old behaviour, use wc\_level. See section 3.3.4 about water clouds for a realistic example how the contents of the wc\_file are converted to optical properties.

#### wc files

A way to specify cloud extinction coefficient, single scattering albedo, and scattering phase function for each layer.

```
wc_files file
```

The file specified by wc\_files 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 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 single scattering albedo of the layer.

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

Note that if using the rte\_solver cdisort or rte\_solver fdisort2 it makes good sense to make the number of moments larger than nstr because all moments are used in the calculation. For rte\_solver fdisort1 and rte\_solver polradtran the number of moments included in the calculations will be nstr+1. Higher order moments will be ignored for these solvers. Please note that the uppermost line of the wc\_files 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\_ipa

Independent column calculation for a 3D cloud field.

```
wc_ipa file
```

As argument a name of a 3D cloud file must be given. This file has to be in the format as needed by MYSTIC, see mc\_wcloud\_file. See examples/UVSPEC\_WC\_IPA.INP for an example.

### wc\_ipa\_files

A two-column file, defining water cloud property files (see wc\_file) in the first column and the corresponding weights in the second column.

```
wc_ipa_files file
```

The radiative transfer calculation is performed independently for each cloud column and the result is the weighted average of all independent columns. If ic\_ipa\_files and wc\_ipa\_files are both defined, both must have the same columns in the same order, otherwise uvspec will complain. See examples/UVSPEC\_WC\_IPA\_FILES.INP for an example.

#### wc\_layer

Interpret cloud properties as layer properties (this is the default behaviour since version 1.4; see also  $wc_file$ ). Cloud 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. For example, 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.

### wc\_level

Interpret cloud properties as level properties (this was the default behaviour before version 1.4; see also wc\_file). If wc\_level is defined, a wc\_file would be interpreted as follows:

```
LWC
                   R\ensuremath{\mbox{\sc eff}}
        (g/m^3) (um)
(km)
 5.000
             0
                        0
 4.000
            0.2
                     12.0
 3.000
            0.1
                     10.0
 2.000
                      8.0
            0.1
```

The value 0.2 g/m<sup>3</sup> 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.

### wc\_no\_scattering

Switch off scattering by water clouds.

### wc\_properties

Possible choices for type are

#### hu

Parameterization by Hu and Stamnes (1993); this is the default setting. Note that the parameterization is somewhat different for correlated\_k 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 correlated\_k; the tables are expected in data\_files\_path/correlated\_k/.../.

For spectral or pseudo-spectral (correlated\_k sbdart) calculations, a set of pre-calculated tables is also available. For spectral or pseudo-spectral calculations wc\_properties\_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).

### wc\_properties\_interpolate

Interpolate water cloud optical properties over wavelength; useful for precalculated optical property files defined with wc\_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).

### wc\_saturate

Obsolete option.

### wc\_scale\_gg

Scale the water cloud asymmetry factor for all wavelengths and altitudes with a float between 0.0 and 1.0.

wc\_scale\_gg value

#### wc scale ssa

Scale the water cloud single scattering albedo for all wavelengths and altitudes with a float between 0.0 and 1.0.

```
wc_scale_ssa value
```

### wc\_scale\_tau

Scale the water cloud optical thickness for all wavelengths and altitudes. with a float between 0.0 and 1000000.0. Also works for 3d clouds.

```
wc_scale_tau value
```

### wc\_set\_gg

Set the water cloud asymmetry factor for all wavelengths and altitudes to 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 a wc\_files. It doesn't make sense to modify only the first moment of an explicit phase function.

```
wc_set_gg value
```

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.

## $wc\_set\_ssa$

Set the water cloud single scattering albedo for all wavelengths and altitudes to a float between 0.0 and 1.0.

```
wc_set_ssa value
```

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.

# wc\_set\_tau

Set the total water cloud optical thickness to a constant value for all wavelengths.

```
wc_set_tau value
```

The optical thickness defined here is the integral from the surface at the userdefined 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.

#### wc set tau550

Set the water cloud optical thickness at 550nm.

```
wc_set_tau550 value
```

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.

#### wvn

Deprecated option. Same as wavelength.

#### 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 0.730km (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. Note that for rte\_solver polradtran the atmosphere file must contain the altitudes specified by zout. 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, dens\_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 dens\_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 (tracegases, temperature ...) are interpolated to the levels introduced by zout, and optical properties are determined from the interpolated atmospheric properties. If heating\_rate, rte\_solver polradtran, rte\_solver rodents, or rte\_solver twostrebe 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.

### 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.

#### 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

$$n(r) = ar^{\alpha} \exp(-br), \tag{6.12}$$

where  $\alpha$  is the distribution parameter given as second argument. (a and b are determined automatically.) The effective radius of the distribution is  $r_{\rm eff} = (\alpha + 3)/b$ . A typical value for water clouds is  $\alpha = 7$ . For ice clouds a typical value is  $\alpha = 1$ . A large value of  $\alpha$  gives close to a monodisperse distribution.

## **LOGNORMAL**

The lognormal distribution of cloud droplet sizes is

$$n(r) = -\frac{a}{r} \exp\left(\frac{-\ln(r/r_0)^2}{2\sigma^2}\right),\tag{6.13}$$

where  $r_0$  is the logarithmic mode of the distribution (calculated automatically) and  $\sigma$  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 <code>libsrc\_f/MIEV.doc</code> and the NCAR Mie report at <code>ftp://climate1.gsfc.nasa.gov/wiscombe/Single\_Scatt/Homogen\_Sphere/Exact\_Mie/</code>

#### mimcut

(positive) value below which imaginary refractive index is regarded as zero (computation proceeds faster for zero imaginary index). Only used by mie\_program MIEVO.

```
mimcut value
```

### nmom

Number of moments of the phase function to be calculated (default: 0).

```
nmom value
```

Only possible with mie\_program MIEVO.

### 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.

### 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  $r_{\rm eff}$ . The default is 5, which means that the size distribution is cut off at a value of  $5 \cdot r_{\rm eff}$ . This value should be increased if only small  $r_{\rm eff}$  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\_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<sup>3</sup>/m<sup>3</sup>], if a 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\_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 MIEVO.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

$$p(\mu) = \sum_{m=0}^{\infty} (2m+1) \cdot k_m \cdot P_m(\mu)$$
 (6.14)

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 uvspecoptions 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

## 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
```

First calculations is done with radius\_min, which will be increased by radius\_step until radius max is reached.

#### 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 of W. Wiscombe.

#### water

The complex refractive index is taken from the REFWAT function of W. Wiscombe.

#### 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
```

Temperature dependence is only considered above 10 micron (water) and 167 micron (ice), respectively. Default: 300K.

#### 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).

#### 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, 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.

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