The radiative transport equation solvers within uvspec

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1 Introduction

The *uvspec* tool includes numerous solvers for the radiative transport equation. To select the appropriate solver for a specific problem may be difficult because it is hard to aquire knowledge of the advantages and limitations of the various solvers. The aim of the present document is to help the user pick the best solver for the given problem by

- presenting the radiative transfer equation in its most general form
- describing the various approximations invoked to solve the equation
- describing each solver and the approximations they are based on.

The number of equations in the two first sections may be intimidating even for the brave-hearted. If you just want to get things done and wonder if *uvspec* includes a solver that may be used for your problem, jump directly to section 4.

2 The radiative transfer equation

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

$$\frac{\partial f}{\partial t} + \nabla_{\mathbf{r}}(\mathbf{v}\ f) + \nabla_{\mathbf{p}}(\mathbf{F}\ f) = Q(\mathbf{r}, \hat{n}, \nu, t). \tag{1}$$

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

$$f(\mathbf{r}, \hat{n}, \nu, t)\ c\ \hat{n} \cdot d\mathbf{S}\ d\Omega\ d\nu\ dt \tag{2}$$

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

$$\nabla_{\mathbf{r}}(\mathbf{v}\ f) = f\ \nabla_{\mathbf{r}}\mathbf{v} + \mathbf{v} \cdot \nabla f = \mathbf{v} \cdot \nabla f, \tag{3}$$

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

where **r** and **v** are independent variables, Eq. 1 may be written as

$$\frac{\partial f}{\partial t} + c\,(\hat{n}\cdot\nabla)\,f = Q(\mathbf{r},\hat{n},\nu,t) \tag{4}$$

where the **r** subscript on the gradient operator ∇ has been omitted.
The differential energy associated with the photon distribution is

$$dE = c\,h\nu\;f\;\hat{n}\cdot d\mathbf{S}\;d\Omega\;d\nu\;dt. \tag{5}$$

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

$$dE = I(\mathbf{r},\hat{n},\nu,t)\;dS\;\;\cos\theta\;d\Omega\;d\nu\;dt, \tag{6}$$

which gives

$$I(\mathbf{r},\hat{n},\nu,t) = c\,h\nu\;f(\mathbf{r},\hat{n},\nu,t). \tag{7}$$

In a steady state situation Eq. 4 may then be written as

$$(\hat{n}\cdot\nabla)\;I(\mathbf{r},\hat{n},\nu) = h\nu\;Q(\mathbf{r},\hat{n},\nu). \tag{8}$$

Eq. 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.

2.1 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.

2.1.1 Cartesian geometry - plane-parallel atmosphere

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

$$\hat{n}\cdot\nabla = n_x\frac{\partial}{\partial x} + n_y\frac{\partial}{\partial y} + n_z\frac{\partial}{\partial z} = \cos\phi\sqrt{1-\mu^2}\frac{\partial}{\partial x} + \sin\phi\sqrt{1-\mu^2}\frac{\partial}{\partial y} + \mu\frac{\partial}{\partial z}, \tag{9}$$

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

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

$$\hat{n} \cdot \nabla = \mu \frac{\partial}{\partial z}. \tag{10}$$

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

2.1.2 Spherical geometry - pseudo-spherical atmosphere

In spherical geometry the streaming term becomes[2]

$$\begin{aligned} \hat{n} \cdot \nabla &= \mu \frac{\partial}{\partial r} + \frac{1-\mu^2}{r} \frac{\partial}{\partial \mu} \\ &+ \frac{\sqrt{1-\mu^2}\sqrt{1-{\mu_0}^2}}{r} \left[\cos(\phi - \phi_0) \frac{\partial}{\partial \mu_0} + \frac{\mu_0}{1-\mu_0^2} \sin(\phi - \phi_0) \frac{\partial}{\partial(\phi - \phi_0)} \right]. \end{aligned} \tag{11}$$

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

$$\hat{n} \cdot \nabla = \mu \frac{\partial}{\partial r} + \frac{1-\mu^2}{r} \frac{\partial}{\partial \mu}. \tag{12}$$

Dahlback and Stamnes (1991) has shown that for mean intensities it is sufficient to include only the first term in Eq. 12 for solar zenith angles up to 90°. Thus,

$$\hat{n} \cdot \nabla = \mu \frac{\partial}{\partial r}. \tag{13}$$

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

2.2 The source term

The source term on the right hand side of Eq. 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

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

be written as[3]

$$\begin{aligned} h\nu\, Q(r,\hat{n},\nu) &= h\nu\, Q(r,\theta,\phi,\nu) = -\beta^{ext}(r,\nu)\; I(r,\theta,\phi,\nu) \\ &+\frac{1}{4\pi}\int_0^\infty \beta^{sca}(r,\nu,\nu')\int_0^{2\pi} d\phi' \int_0^{\pi} d\theta' p(r,\theta,\phi;\theta',\phi') I(r,\theta',\phi',\nu')d\nu' \\ &+\beta^{abs}(r,\nu)\; B[T(r)]. \end{aligned} \tag{14}$$

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

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

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

$$\beta^{abs}(r,\nu) = \sum_i \beta_i^{abs}(r,\nu), \qquad \beta_i^{abs}(r,\nu) = n_i(r)\sigma_i^{abs}(\nu) \tag{15}$$

$$\beta^{sca}(r,\nu) = \sum_i \beta_i^{sca}(r,\nu), \qquad \beta_i^{sca}(r,\nu) = n_i(r)\sigma_i^{sca}(\nu) \tag{16}$$

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

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

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

where the phase function for each species

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

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

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

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

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

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.

2.3 The radiative transfer equation in 1D

In plane-parallel geometry the monochromatic[5] radiative transfer equation 8 is written by combining Eq. 10 and Eq. 14

$$\begin{aligned} -\mu\frac{dI(z,\mu,\phi)}{\beta^{ext}dz} &= I(z,\mu,\phi) \\ &-\frac{\omega(z)}{4\pi}\int_0^{2\pi}d\phi'\int_{-1}^{1}d\mu' p(z,\mu,\phi;\mu',\phi')I(z,\mu',\phi') \\ &-(1-\omega(z))B[T(z)] \end{aligned} \quad (17)$$

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. 17, but with z replaced by r.

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 $\mathbf{I}$

$$\mathbf{I} = (I,Q,U,V), \quad (18)$$

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

The degree of polarization p is defined as

$$p = \frac{\sqrt{Q^2+U^2+V^2}}{I}. \quad (19)$$

[5]Frequency redistribution is required if Raman scattering is included in the calculation. For many applications Raman scattering is negligible and the photons are assumed not to change frequency. They are monochromatic. Thus, all frequency dependence have been suppressed in Eq. 17.

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

$$p_{lin} = \frac{\sqrt{Q^2 + U^2}}{I}, \tag{20}$$

and the the degree of circular polarization is defined as

$$p_{circ} = \frac{V}{I}. \tag{21}$$

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.

3 General solution considerations

A multitude of methods exist to solve the radiative transfer equation 8. Most methods have some commonalities and they are briefly described below.

3.1 Direct beam/diffuse radiation splitting

The integro-differential radiative transfer equation 8 gives the radiance field when solved with appropriate boundary conditions, that is, the radiation incident at the bottom and the top of the atmosphere. At the bottom of the atmosphere the Earth partly reflects radiation and also emits radiation as a quasi-black-body. At the top of the atmosphere ($z = z_{\text{toa}}$) a parallel beam of sunlight with magnitude I^0 in the direction μ_0 may be present

$$I(z_{\text{toa}}, \mu) = I^0 \delta(\mu - \mu_0), \tag{22}$$

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 8 is already inhomogeneous, the addition of another inhomogeneous term does not necessarily complicate the problem. Hence the intensity field is written as the sum of the direct (dir) and the scattered (sca)(or diffuse) radiation

$$I(z, \mu, \phi) = I^{\text{dir}}(z, \mu_0, \phi_0) + I^{\text{sca}}(z, \mu, \phi), \tag{23}$$

where μ_0 and ϕ_0 are the solar zenith and azimuth angles respectively. Inserting Eq. 23 into Eq. 8 it is seen that the direct beam satisfies

$$-\mu\frac{dI^{\rm dir}(z,\mu_0,\phi_0)}{\beta^{ext}dz} = -\mu\frac{dI^{\rm dir}(z,\mu_0,\phi_0)}{d\tau} = I^{\rm dir}(z,\mu_0,\phi_0) \tag{24}$$

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

$$\begin{aligned}-\mu\frac{dI(\tau,\mu,\phi)}{d\tau} &= I(\tau,\mu,\phi)\\ &-\frac{\omega(r)}{4\pi}\int_0^{2\pi}d\phi'\int_{-1}^{1}d\mu' p(\tau,\mu,\phi;\mu',\phi')I(\tau,\mu',\phi)\\ &-(1-\omega(\tau))B[T(\tau)]\\ &-\frac{\omega(\tau)I^0}{4\pi}p(\tau,\mu,\phi;\mu_0,\phi_0)e^{-\tau/\mu_0}.\end{aligned} \tag{25}$$

Solution of Eq. 24 for the direct beam yields the Beer-Lambert-Bouguer law

$$I^{dir}(\tau,\mu_0) = I^0\ e^{-\tau/\mu_0}. \tag{26}$$

The popular **disort** solver (Stamnes et al., 1988, 2000) solves Eqs. 24-25.

3.2 Pseudo-spherical approximation

In the pseudo-spherical approximation the extinction path τ/μ_0 in Eqs. 25 and 26 is replaced by the Chapman function, $ch(r,\mu_0)$ (Rees, 1989; Dahlback and Stamnes, 1991)

$$ch(r_0,\mu_0) = \int_{r_0}^{\infty}\frac{\beta^{ext}(r,\nu)\ dr}{\sqrt{1-\left(\frac{R+r_0}{R+r}\right)^2(1-\mu_0^2)}}. \tag{27}$$

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

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

$$I^{dir}(r,\mu) = I^0\ e^{-ch(r,\mu_0)} \tag{28}$$

and the diffuse radiation is approximated by replacing the plane-parallel direct beam source in Eq. 25 with the corresponding direct beam source in spherical geometry

$$\begin{aligned}-\mu\frac{dI(\tau,\mu,\phi)}{d\tau} &= I(\tau,\mu,\phi)\\ &-\frac{\omega(r)}{4\pi}\int_0^{2\pi}d\phi'\int_{-1}^{1}d\mu' p(\tau,\mu,\phi;\mu',\phi')I(\tau,\mu',\phi)\\ &-(1-\omega(\tau))B[T(\tau)]\\ &-\frac{\omega(\tau)I^0}{4\pi}p(\tau,\mu,\phi;\mu_0,\phi_0)e^{-ch(\tau,\mu_0)}.\end{aligned} \tag{29}$$

The **sdisort** solver included in the libRadtran software package (Mayer and Kylling, 2005) solves Eqs. 28-29.

3.3 Boundary conditions

The diffuse radiative transfer Eq. 25 is solved subject to boundary conditions at the top and bottom of the atmosphere. At the top boundary there is no incident diffuse intensity[6] ($\mu \geq 0$)

$$I(\tau = 0, -\mu, \phi) = 0. \tag{30}$$

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

$$\begin{aligned} I(\tau = \tau_g, \mu, \phi) &= \epsilon(\mu)B[T(\tau_g)] + \frac{1}{\pi}\mu_0 I_0 e^{-\tau_g/\mu_0}\rho(\mu, \phi; -\mu', \phi') \\ &+ \frac{1}{\pi}\int_0^{2\pi} d\phi' \int_0^1 \rho(\mu, \phi; -\mu', \phi') I(\tau, -\mu', \phi')\mu' d\mu', \end{aligned} \tag{31}$$

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

In the case of a Lambertian reflecting bottom boundary with albedo $\rho(\mu, \phi; -\mu', \phi') = A$, Eq. 31 simplifies to

$$\pi I(\tau_L, \mu) = \pi\ \epsilon\ B[T(\tau_g)] + \mu_0\ A\ I^0 e^{-\tau_g/\mu_0)} + 2\pi\ A \int_0^{2\pi} d\phi' \int_0^1 \mu I(\tau_L, -\mu, \phi) d\mu. \tag{32}$$

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. 31 and 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

3.4 Separation of the azimuthal Φ-dependence, Fourier decomposition

For scattering processes in the atmosphere the scattering phase function depends only on the angle Θ between the incident and scattered beams. This may be used to seperate out the Φ-dependence in Eqs. 25 and 29 as follows. The phase function is first expanded as a series of Legendre polynomials

$$p(\tau, \mu, \phi; \mu', \phi') = p(\tau, \Phi) = \sum_{l=0}^{2M-1} (2l + 1) g_l(\tau) p_l(\cos\Phi) \tag{33}$$

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

where the phase function moments g_l are given by

$$g_l(\tau) = \frac{1}{2}\int_{-1}^{+1} p_l(\cos\Phi)p(\tau,\Phi)d(\cos\Phi). \tag{34}$$

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. 33 gives

$$p(\tau,\Phi) = \sum_{l=0}^{2M-1}(2l+1)g_l(\tau)\left\{p_l(\mu)p_l(\mu') + 2\sum_{m=1}^{l}\Lambda_l^m(\mu)\Lambda_l^m(\mu')\cos m(\phi-\phi')\right\} \tag{35}$$

where the normalized associated Legendre polynomials are defined as

$$\Lambda_l^m(\mu) = \sqrt{\frac{(l-m)!}{(l+m)!}}P_l^m(\mu), \tag{36}$$

and $P_l^m(\mu)$ are the standard Legendre polynomials. The cosine dependence of the phase function, Eq. 35, suggests that cosine expansion of the intensity may be fruitful. Expanding the intensity as a cosine Fourier series:

$$I(\tau,\mu,\phi) = \sum_{l=0}^{2M-1} I^m(\tau,\mu)\cos m(\phi_0-\phi) \tag{37}$$

and inserting into Eqs. 25 and 29 gives $2M$ independent integro-differential equation (only the plane-parallel version is shown here)

$$\begin{aligned} -\mu\frac{dI^m(\tau,\mu)}{d\tau} &= I^m(\tau,\mu) \\ &-\frac{\omega(r)}{2}\int_{-1}^{1}d\mu'\sum_{l=m}^{2M-1}(2l+1)g_l(\tau)\Lambda_l^m(\mu)\Lambda_l^m(\mu')I^m(\tau,\mu') \\ &-\delta_{m0}(1-\omega(\tau))B[T(\tau)] \\ &-\frac{\omega(\tau)I^0}{4\pi}(2-\delta_{m0})\sum_{l=m}^{2M-1}(2l+1)g_l(\tau)\Lambda_l^m(\mu)\Lambda_l^m(\mu')e^{-\tau/\mu_0}. \end{aligned} \tag{38}$$

where

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

3.5 Calculated quantities

Solution of the radiative transfer equation generally yields the diffuse radiance

$$I(\tau, \mu, \phi) \tag{39}$$

and the direct radiance

$$I^{\mathrm{d}ir}(\tau, \mu_0, \phi_0). \tag{40}$$

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

$$E^+(\tau) = \int_0^{2\pi} d\phi \int_0^1 \mu I(\tau, \mu, \phi) d\mu \tag{41}$$

$$E^-(\tau) = \mu_0 I_0 e^{-\tau/\mu_0} + \int_0^{2\pi} d\phi \int_0^1 \mu I(\tau, -\mu, \phi) d\mu. \tag{42}$$

Furthermore, the mean intensity

$$\overline{I}(\tau) = \frac{1}{2\pi}\left[I_0 e^{-\tau/\mu_0} + \int_0^{2\pi} d\phi \int_0^1 I(\tau, -\mu, \phi) d\mu + \int_0^{2\pi} d\phi \int_0^1 I(\tau, \mu, \phi) d\mu\right], \tag{43}$$

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

$$F(\tau) = 4\pi\overline{I}(\tau). \tag{44}$$

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

$$\frac{\partial T}{\partial t} = -\frac{4\pi}{c_p \rho_m}\frac{\partial E}{\partial z} = -\frac{4\pi}{c_p \rho_m}(1-w)(\overline{I} - B)\frac{\partial \tau}{\partial z}. \tag{45}$$

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

The various solvers have different capabilities to calculate the above radiative quantities. The user is referred to section 4 for a brief overview of the different solvers included in *uvspec* and their respective capabilities. For a complete description of all solvers with options the *uvspec* User's Guide and Mayer and Kylling (2005) may 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.

3.6 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 are 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 cloud 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.

4 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 1.

4.1 DIScrete ORdinate Radiative Transfer solvers (DISORT)

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

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

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

4.1.1 DISORT solvers (disort, disort2, disort2_original)

This group of solvers solve the 1D plane-parallel radiative transfer equation 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*.

disort The original DISORT version 1.3.

disort2 The DISORT version 2.0 with improved treatment of the phase function.

disort2_original The original DISORT version 2.0.

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.

If you are in doubt, use the modified version 2.0. The default RTE solver in *uvspec* is **disort2**. Note that these solvers assumes a flat Earth (planet). If you are worried about spherical effects please consider the pseudo-spherical version of DISORT included in *uvspec*.

4.1.2 Pseudo-spherical DISORT (sdisort, spsdisort)

Dahlback and Stamnes (1991) extended the DISORT version 1.3 solver to pseudo-spherical geometry by solving equation 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.

4.1.3 General source term (qdisort)

The **qdisort** solver is similar to **sdisort** with the addition of a general source term to the right in Eq. 29. It is only used when Raman scattering is included the calculation.

4.1.4 Two-stream solvers (twostr, twostrpp)

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 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.

4.2 Monte Carlo and MYSTIC (montecarlo)

The Monte Carlo method is the most straightforward way to calculate 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.

In order to calculate (polarized) radiances for cloudy atmospheres accurately several "tricks" are required in order to speed up the calculations, for instance 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.

Originally, the Monte Carlo solver MYSTIC was developed as a forward tracing method for the calculation of irradiances and radiances in 3-D plane-parallel atmospheres. The model has been extended to include spherical geometry and a backward tracing mode (Emde and Mayer, 2007). Recently, the model has been further extended to include polarized radiation due to scattering by randomly oriented particles, i.e. clouds, aerosols, and molecules (Emde et al., 2009). For general questions about 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). A detailed introduction to the Monte Carlo technique and in particular to MYSTIC is given in Mayer (2009).

4.3 Polarization (polradtran)

The **polradtran** solver developed by Evans and Stephens (1991) solves the plane-parallel RTE including polarization.

4.4 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

$$-\mu \frac{dI(z,\mu,\phi)}{\beta^{ext} dz} = I(z,\mu,\phi) - (1-\omega(z))B[T(z)] \qquad (46)$$

where $I(z,\mu,\phi) = I(z,\mu,\phi,\nu)$ represents the spectral radiance at the wavenumber ν, $\omega(z) = \omega(z,\nu)$ 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.

4.5 Solar single scattering (sss)

The **sss** solver solves the scalar RTE for single scattered radiation in a 1D plane-parallel atmmosphere. It includes solar radiation. Radiation is only output at the top of the atmosphere radiance as a function of μ and ϕ.

4.6 Solar single scattering (sssi)

Similar to the **sss** solver, but includes a correction for reflecting cloud layers. It currently only works for nadir radiance.

Table 1: The various radiative transfer equation (RTE) solver currently in uvspec.

RTE solver	Geometry	Radiation quantities	Reference	Comments
DISORT 1.3	1D, PP	E, F, L	Stamnes et al. (1988)	multi-stream discrete ordinate
DISORT 2.0	1D, PP	E, F, L	Stamnes et al. (2000)	multi-stream 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 for low sun angles;
twostrpp	1D, PS	E, F	Kylling et al. (1995)	plane-parallel version of twostr;
sdisort	1D, PS	E, F, L	Dahlback and Stamnes (1991)	pseudo-spherical correction for low sun angles; double precision, customized for airmass calculations based on DISORT 1.3
spsdisort	1D, PS	E, F, L	Dahlback and Stamnes (1991)	pseudo-spherical correction for low sun angles; single precision, not suitable for cloudy conditions
qdisort	1D, PS	E, F, L		based on sdisort, includes extra source term used for Raman scattering;
tzs	1D, PP	L(TOA)		thermal, zero scattering
sss	1D, PP	L(TOA)		solar, single scattering
montecarlo	3D, PP 1D, S	**E, F, L**	Mayer (2009); Emde and Mayer (2007) Emde et al. (2009)	Monte Carlo[a]

[a] not included in the free package; available in joint projects

Explanation:	PP, plane-parallel	E, irradiance
	S, spherical	F, actinic flux
	PS, pseudo-spherical	F, actinic flux
	1D, one-dimensional	L, radiance
	3D, three-dimensional	L(TOA), radiance at top of atmosphere

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

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