Towards a Generic Radiative Transfer Model for the Earth's Surface-Atmosphere System: ESAS-Light

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WP2300:

Development plan for libRadtran demonstration version

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1 Introduction

This development plan includes work plans for the implementation of Raman scattering and polarization. Other smaller work packages like the improvement of aerosol and surface handling, the coupling of *libRadtran* with a line-by-line model and the implementation of a graphical user interface are also adressed. Equations referenced in this document are found in the document "Towards a Generic Radiative Transfer Model for the Earth's Surface-Atmosphere System: ESAS-Light, ESTEC Contract No AO/1-5433/07/NL/HE, WP2200: Algorithm theoretical basis documents for libRadtran demonstration version" (Kylling and Emde, 2008).

2 WP3100 - Raman scattering

The inclusion of Raman scattering consists of several parts. The optical properties of the scattering process must be correctly and efficienty calculated and the radiative transfer equation appropriately solved. Furthermore, the wavelength resolution of the calculation must be considered. Finally, everything must be validated. Below the development plan for the different parts is outlined. Validation is discussed both for each part and for the final product.

2.1 Cross section and phase function

The Raman scattering cross section, Eq. 1, may be readily calculated utilizing Eqs. 2-8 and 10-12. There are no specific problems involved in implementing these formulas into uvspec. It is noted that the calculation of the Placzek-Teller coefficients is simplified for N_2. The implementation will be such that more accurate coefficients may readily be adopted at a later stage.

The calculation of the Raman scattering cross section will be validated against earlier published results, see, for example, Joiner et al. (1995, Fig. 3), Sioris and Evans (1999, Fig. 1), and Spurr et al. (2008, Fig. 1).

The implementation of the Raman scattering phase function Eq. 13 poses no problems. It will be validated by plotting and visual inspection.

2.2 Radiative transfer equation solver

The uvspec tool solves the monochromatic radiative transfer equation, Eq. 14. To implement the first-order Raman scattering correction to uvspec, a separate loop over wavelength must be introduced into uvspec. During the first execution of the loop the zeroth order Eq. 14 is solved. The first order correction Eq. 19, is solved during the second and last iteration.

The new loop over wavelength will require the introduction of some temporary arrays to store information for each iteration. Also, new arrays for the Raman scattering cross section and phase function have to be added.

The calculation of the source term, Eq. 31, requires quadrature angles, μ_i, and weights, c_i. Also, the appropriate Legendre polynomials are needed for the calculation of the phase function. All

these quantities are currently calculated internally in each radiative transfer equation solver. For the source term these quantities will be have to calculated separately outside of the solver. As this is already done in separate functions inside the solvers it is no major problem doing this outside of the solvers. In addition, the transmission term, $e^{-T(\tau_\lambda)}$, has to be calculated. This should also pose no major problem as the optical depth τ is available outside the solver.

The validation of the implementation of the general source term will be done in two steps:

- The general source term will be set equal to the direct beam source. It should thus give the same results as the direct beam source and ensure the correct implementation of the general source term.
- To validate the redistribution of photons over wavelength, an artifical spectrum with a single absorption line will be input to uvspec. The number of photons which are filled in should equal to the number of photons taken from nearby wavelengths. This test will ensure the conservation of photons by the code.

2.3 Spectral resolution

To accurately simulate the effect of Raman scattering a high spectral resolution is required due to the large number of lines involved within about ± 2 nm of the spectral line of interest. This implies that both memory requirements and computational time may be substantial. If this turns out to be a real problem it is possible to perform opimalization over wavelength using the so-called "binning realization" of Spurr et al. (2008).

2.4 Validation

A few authors have published results comparing model and measurements line filling-in of Fraunhofer and absorption due to Raman scattering, see for example Joiner et al. (1995); Spurr et al. (2008). These sources will be scrutinized for availability of input and output data for which the present implementation may be compared.

Finally, we will check the implementation against surface UV measurements earlier published by participants of this project (Mayer et al., 1997, 1998).

2.5 Responsibility and schedule

Raman scattering will be implemented by Arve Kylling. A first version will be available at the MTR meeting (KO+12M) and the final validated version at PM4 (KO+18M).

3 WP3200 - Polarisation

3.1 Implementation in MYSTIC

Additions that are required in order to implement polarization by Rayleigh, aerosol, and cloud scattering into the Monte Carlo model MYSTIC are described in the following sections:

3.1.1 Photon initialization

In the scalar Monte Carlo models photons are traced and associated with photon weights. The weight accounts for absorption and in the local estimate technique it is the probability that the photon is scattered into a certain direction. To implement polarization, a weight vector corresponding to the Stokes components is associated to each photon. The initial weight vector to simulate solar radiative transfer is $\mathbf{w} = (1, 0, 0, 0)$, corresponding to the unpolarized extraterrestrial solar radiation. In the following the photon weight vector is called Stokes vector. The initial direction of the photon $\hat{\mathbf{n}}_\mathbf{0}$ is defined by the solar zenith angle for solar radiative transfer.

3.1.2 Sampling the pathlength

The sampling of the pathlength of the photon is equivalent to the scalar model. The transmission T is defined as

$$T = \exp(-\int_0^s \beta_{\text{ext}} s' ds') = \exp(-\tau) \tag{1}$$

where β_{ext} is the extinction coefficient, s the distance and τ the optical thickness. The extinction coefficient is computed from the extinction cross section (Eq. 53) by multiplication with the particle number density. The transmission may be interpreted as the probability that the photon travels the distance τ without interactions.

3.1.3 Scattering (randomly oriented particles or Rayleigh)

For randomly oriented particles the phase matrix is usually calculated in the scattering coordinate frame, which is defined by the incoming direction, the scattering direction, and a vector orthogonal to those directions. The advantage of using the scattering frame is that the phase matrix and the extinction matrix depend only on the scattering angle. In order to apply the phase matrix correctly the Stokes vector needs to be rotated into the respective scattering frame for each scattering event. This can be realized as follows:

- Sample a random number between 0 and 2π for the azimuthal direction ϕ_i, which is isotropic for randomly oriented particles.
- The scattering frame of the first scattering event is defined by $\hat{\mathbf{n}}_\mathbf{0}$, $\hat{\mathbf{n}}_{\boldsymbol{\phi}\mathbf{1}}$ (a normal vector orthogonal to $\hat{\mathbf{n}}_\mathbf{0}$ in the direction of ϕ_1) and $\hat{\mathbf{n}}_{\perp\mathbf{1}} = \hat{\mathbf{n}}_\mathbf{0} \times \hat{\mathbf{n}}_{\boldsymbol{\phi}\mathbf{1}}$ (a normal vector orthogonal to the scattering plane).

- Rotate the Stokes vector into the scattering frame by applying the Stokes rotation matrix (Eq. 61). The rotation angle is the angle between the orthogonal of the scattering plane and the z-direction of the model coordinate system:

$$\alpha_1 = \arccos(\hat{\mathbf{n}}_{\perp\mathbf{1}} \cdot \hat{\mathbf{n}}_{\mathbf{z}}) \tag{2}$$

  In case of multiple scattering the Stokes vector is rotated from the scattering frame of the previous scattering event to the new scattering frame. For the i^{th} scattering event the rotation angle is

$$\alpha_i = \arccos(\hat{\mathbf{n}}_{\perp\mathbf{i}} \cdot \hat{\mathbf{n}}_{\perp\mathbf{i-1}}) \tag{3}$$

  where

$$\hat{\mathbf{n}}_{\perp\mathbf{i}} = \hat{\mathbf{n}}_{\mathbf{i-1}} \times \hat{\mathbf{n}}_{\phi\mathbf{i}} \tag{4}$$

- Now the scattering cross sections for all particles and molecules that are present at the interaction point can be calculated according to Eq. 54. These are multiplied with the number densities to obtain the scattering coefficients, which are used to decide which interaction takes place. For instance, if there are cloud droplets and molecules in the model atmosphere, we may use a random number $r \in [0, 1]$ to decide whether the photon interacts with a cloud droplet or a molecule. If the random number is smaller than the ratio between the Rayleigh scattering coefficient and the total scattering coefficient, the photon interacts with the molecule:

$$r \leq \frac{\beta_{\text{sca,r}}}{\beta_{\text{sca,r}} + \beta_{\text{sca,c}}} \tag{5}$$

  Here $\beta_{\text{sca,r}}$ is the Rayleigh scattering coefficient and $\beta_{\text{sca,c}}$ is the cloud scattering coefficient. Else, if the random number is larger than this ratio the photon interacts with the cloud droplet.

- The phase function is calculated according to Eq. 57 and can be used as probability density function to sample the scattering angle Θ_i.

- To calulate the scattered Stokes vector $\mathbf{I}_\mathbf{i}^\mathbf{sca}$ the phase matrix $\mathbf{P}(\Theta_i)$ is multiplied with the incoming Stokes vector $\mathbf{I}_\mathbf{i}^\mathbf{inc}$:

$$\mathbf{I}_\mathbf{i}^\mathbf{sca} = \mathbf{P}(\Theta_i)\mathbf{I}_\mathbf{i}^\mathbf{inc} \tag{6}$$

When the photon is counted at the end of its journey the associated Stokes vector is rotated to the model coordinate frame (x, y, z) in order to obtain the final result.

3.1.4 Scattering (arbitrarily oriented particles)

If the particles are arbitrarily oriented, the phase matrix can only be calculated in the model coordinate frame (x, y, z). In this case we can use the phase function (Eq. 57) as probability

density function to sample both angles, Θ and ϕ. We do not need to rotate the Stokes vector into the scattering frame.

The major practical difficulty in calculating polarization of arbitrarily oriented particles is, that the phase matrix depends on four angles (incoming and scattered directions), as well as on the wavelength and on the effective radius and requires a huge amount of computational memory. The same argument applies for the extinction matrix and the absorption vector. For this reason, we will first concentrate on the case of randomly oriented particles, which is in most cases a realistic assumption.

3.2 Include tools to calculate scattering by aspherical particles

To perform polarized radiative transfer simulations, single scattering properties of cloud particles are required, i.e. the 4x4 phase matrix, the 4x4 extinction matrix, and the 4 component absorption vector (for each possible particle size, shape, and orientation).

The well-tested Mie-code by Wiscombe (1980), which is already incuded in the *libRadtran* package (Mie-tool), can be used to generate the data for spherical particles, i.e. water droplets or some aerosol types. *libRadtran* does not include a tool to calculate scattering properties of aspherical particles. The first step in this study is to test freely available codes for computing scattering properties of aspherical particles which can be randomly oriented or horizontally aligned (which is often observed in cirrus clouds). Based on these tests the best code will be implemented as a tool in the *libRadtran* toolbox. Parameterizations of scattering properties are not available for polarized radiative transfer, so it is absolutely necessary to have such a tool.

3.3 Generate database for single scattering properties

The objective of this task is to generate a database of single scattering properties of cloud particles to be used for polarized calculations. The first version of the database to be generated within the project will include only scattering properties of spherical particles. This can be achieved using the already available Mie-tool. The database will be easily extendable for aspherical particles provided that a good tool to calculate scattering properties of aspherical particles is available.

The new database may be used as input to MYSTIC (polarized) and to the fast vector code polradtran by Evans and Stephens (1991).

3.4 Validation

The model will be validated against the well-known and well tested polradtran solver by (Evans and Stephens, 1991), that is already implemented in libRadtran for 1D reference cases. It will also be compared to benchmark results by Collins et al. (1972).

3.5 Responsibility and schedule

Polarization will be implemented by Claudia Emde. A first version will be available at the MTR meeting (KO+12M) and the final validated version at PM4 (KO+18M).

4 WP3300 - Surface properties

4.1 Include additional BRDF data

The BRDF is needed for the correction of view and illumination angle effects of the surface and is therefore an essential input parameter for simulating radiances. The most important effects of the BRDF are the sunglint of water bodies and the hot spot of surfaces with vegetation.

The BRDF options of *libRadtran* will be extended so that the operational MODIS BRDF/albedos data sets for land surface and the parameterisaton of Ebuchi and Kizu (2002) for sea surfaces can be used for radiative transfer simulations with the MYSTIC and DISORT solvers.

4.2 Responsibility and schedule

Enhanced surface properties will be implemented by Ulrich Hamann. A first version will be available at MTR (KO+12M) and the final validated version at PM4 (KO+18M).

5 WP3400 - Aerosol handling

The current *libRadtran* version includes the various aerosol standard models as defined by Shettle (1989). The standard models may be modified by scaling aerosol visibility or the aerosol optical thickness, or by modifying the asymmetry parameter, the single scattering albedo, or the Angström coefficient.

5.1 Mixing of aerosol types

In reality the mixture of different aerosol types can be highly variable. To do a simulation of an aerosol mixture different to the Shettle models, the user can generate an input file containing the optical properties of this mixture. The objective of this task is to extend *libRadtran* in such a way, that a more flexible treatment of aerosols is possible. The user should be able to define an aerosol mixture in the *libRadtran* input file and the mixing should then be done internally by the *libRadtran* program. Implementation of such an option is rather straightforward, the mixing of different aerosol types is done in analogy to mixed phase clouds.

5.2 Aerosol database for polarized radiative transfer based on OPAC

A database of scattering properties of aerosol basic types will be calculated using the Mie tool. As input for the Mie tool, the refractive index of the aerosol and its size distributions are required. This data will be taken from the OPAC database (Hess et al., 1998), which includes the following basic types: water soluble aerosol, soot, sea salt (accumulated and coarse modes), mineral (nucleated, accumulated and coarse modes), transported mineral, sulfate droplets. At completion *libRadtran* will allow the user to define arbitrary mixtures composed of these basic aerosol types. The newly generated aerosol database will include phase matrices, so that the depolarization by aerosols can be calculated using one of the polarized RT solvers (MYSTIC or polradtran).

5.3 Responsibility and schedule

Enhanced aersol properties will be implemented by Claudia Emde. A first version will be available at PM3 (KO+9M) and the final validated version at PM4 (KO+18M).

6 WP3500 - Further Extensions

6.1 Line-by-line interface

Line-by-line calculations are required to accurately simulate absorption lines which are measured by sensors with high spectral resolution. The developement of a line-by-line model is rather complex, so we will use an external open source model to calculate absorption coefficients and provide an interface that reads the output from the external model and converts it to the input format required by libRadtran.

6.1.1 The ARTS line-by-line model

ARTS (Buehler et al., 2005) is an open source line-by-line model which works with arbitrary wavelength grids, hence it can be used both for the simulation of high resolution sensors, and for the simulation of broad frequency ranges. ARTS is a flexible tool that can use arbitrary versions of the HITRAN database. It includes up-to-date absorption continuum models.

To enhance computation speed, ARTS has the option to compute lookup-tables that include absorption coefficients for a reference atmospheric profiles and for perturbations in pressure and temperature. This option is very useful for instance if one like to perform line-by-line simulations for a large number of radiosonde profiles. One needs to do the extensive line-by-line calculation only once to compute the lookup-table, and after that one can extract the absorption coefficients for arbitrary profiles very quickly.

6.1.2 Interface to libRadtran

A python interface has been developed that converts the ARTS output a libRatdran input file. This interface and the respective documentation will be added to the toolbox.

6.1.3 Validation

ARTS has been compared to genln-2 and there was a very good agreement if the same HITRAN database was used. Coupled ARTS-libRadtran radiative transfer calculations have been compared to irradiance measurements in the atmospheric window from 8–12μm. Radiosonde profiles were available as model input. There was a very good agreement between measurements and model simulations. More details will be available in the verification report (D10) of the ESAS-Light study.

6.1.4 Responsibility and schedule

A prototype interface has been developed by Claudia Emde. It will be included in the libRadtran toolbox until PM3 (KO+9M) and the final validated version will be available at PM4 (KO+18M).

6.2 Refraction

Atmospheric refraction is very important for limb sounding instruments where the horizontal path through the atmosphere becomes large. For this reason refraction will be implemented in the MYSTIC model, which can be operated in fully spherical geometry. The implementation of refraction is a straightforward task. Using Snells' law refraction at each grid box boundary in the Monte Carlo model will be calculated. Snell's law of refraction can be written as

$$n_1 \sin \alpha = n_2 \sin \beta \tag{7}$$

Here n_1 and n_2 are the refractive indices of two adjacent model layers and α and β are the angles of the propagation direction with respect to the normal of the interface.

6.2.1 Responsibility and schedule

Refraction will be implemented by Claudia Emde. A first version will be available at the MTR meeting (KO+12M) and the final validated at PM4 (KO+18M).

6.3 Graphical user interface (GUI)

The general functioning of the GUI is to create a uvspec input file in a user-friendly manner, run the uvspec tool with this input file and store the resulting output in a user-specified file. Finally, the GUI should be able to plot the output. As the underlying tool, uvspec, is under continuous

development the GUI must be designed and implemented such that new options and functionality may easily be added. This suggests an incremental development and implementation of the GUI. As such it is appropriate to start with the simplest uvspec input files. Thus, the prototype version of the GUI will include the following functionality:

- The creation and saving of uvspec input files with the options found in the `UVSPEC_SIMPLE.INP` and `UVSPEC_CLEAR.INP` input files. For the later input file only part of the options will be included.
- The execution of the uvspec tool with the loaded uvspec input file. The output is saved to a user specified file.
- The plotting of spectra output when using the above input files.
- For some input options help documentation will be included to demonstrate how this may be implemented.

Although the prototype has limited capabilities it will demonstrate the main functionality of the final product.

6.3.1 Responsibility and schedule

A prototype interface has been developed by Arve Kylling. It will be included in the libRadtran toolbox until PM3 (KO+9M) and the final validated version will be available at PM4 (KO+18M).

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