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

ESTEC Contract No AO/1-5433/07/NL/HE

WP6000: Recommendations for future development of libRadtran

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December 3, 2009

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1 Introduction

The aim of the ESASLight project is to develop a flexible radiative transfer toolbox for the Earth atmosphere-surface system in the solar and thermal spectral ranges.

Radiative transfer models are very important for a better understanding of the Earth-atmosphere system. Solar radiation drives atmospheric circulation and hence weather and climate. Tropospheric and stratospheric chemistry are controlled by photochemical reactions and hence by shortwave radiation. Accurate knowledge about solar and terrestrial radiation and their interaction with clouds, aerosol particles, and trace gases is therefore required for all fields of atmospheric science.

Remote sensing of atmospheric and surface components uses radiation, either from the sun, the atmosphere or an artificial source which is modified along its path through the atmosphere. Radiative transfer modelling plays a key role for remote sensing because it is needed to design remote sensing instruments and to develop and test inversion algorithms. In the scientific community a number of often highly specialized atmospheric radiative transfer (RT) models have been developed each of which emanates from a different set of original requirements. During the development of RT models a trade off has to be made between the computational speed and the accuracy of the model leading to a long list of model simplifications.

The radiative transfer toolbox developed within the ESASLight project should include the most commonly used forward modeling RT tools from the ultraviolet (UV) to the thermal infrared (TIR) spectral domain for the Earth atmosphere-surface system and provide a set of standard radiative transfer tools for the development of ESA commissioned inversion schemes and calibration/validation activities.

As base model the *libRadtran* toolbox (Mayer and Kylling, 2005) has been selected which included many of the requested features and tools. In the currently ongoing ESASLight study the following additions have been included:

- Polarized 3D solver (Emde et al., 2009)
- Raman Scattering
- First version of a graphical user interface (GUI)
- Improved aerosol handling
- Several smaller extensions

The long term objective of the ESASLight project is to give actors in the field of remote sensing of planetary environments full access to a user friendly, open source, well documented and free of charge radiative transfer toolbox. With the *libRadtran* toolbox this objective is already met, but of course such a toolbox is never complete. New measurement techniques (e.g. polarization measurements for remote sensing of ice clouds) require new forward modelling capabilities. Ideas of what could be implemented in a future ESASLight study are given below. Besides new algorithms, the first version of the GUI needs to be improved and extended to include the full *libRadtran* functionality. A *libRadtran* workshop should be organized for *libRadtran* users in order to help new users to get started and to discuss specific problems with experienced users.

2 Work to be performed - Task descriptions

Tasks 1–4 include documentation of the new algorithms, the new databases etc. New algorithms include verification. All tasks should run in parallel, and apart from Task 6 (Dissemination of *libRadtran*), they will start at kick off and end 3 months before the final presentation of the activity.

2.1 Task1 - New algorithms

2.1.1 Rotational Raman scattering

The present implementation of rotational Raman scattering within *libRadtran* works well for the situations it was designed for. However, it has some limitations that may be of concern for some applications. These are listed below in decreasing order of importance

- The current implementation of Raman scattering within the *libRadtran* model agrees well with published results and is thus accurate within the limitations of the comparisons that have been made. However, the present implementation is also slow as it performs all simulations with full spectral resolution. That involves 233 calls to DISORT to calculate the amount of Raman scattered radiation to and from a single wavelength. This number may be reduced by a factor of between 10-20 for single wavelength simulations. The reduction may be achieved by calculating the elastic scattering term at a few selected wavelengths only. For larger spectral regions a speed increase by a factor of about 100 may be expected. The increase in speed will depend on the spectral behaviour of other atmospheric processes such as scattering by aerosol and clouds and absorption by trace gases.

- The present implementation of Raman scattering is one-dimensional. It has recently be shown that 3D clouds may have a 3D effect on the amount of Raman scattered radiation. This may have an effect for example on remote sensing applications that are sensitive to Raman scattering. The *libRadtran* model already includes the MYSTIC 3D Monte Carlo model (Mayer, 2009; Emde and Mayer, 2007). The MYSTIC model may be extended to include Raman scattering to study these effects. Besides being a tool to study 3D effects on Raman scattering, a Monte Carlo implementation may also be used to test the current 1D implementation and vice versa.

- Only single order rotational Raman scattering is included in the present implementation of Raman scattering. If Raman scattering is included in the MYSTIC model it would be both feasible and of interest to include multiple Raman scattering. The effect of multiple Raman scattering has been estimated to be small, but calculations for realistic situations are yet to be made.

The increase in speed of the Raman scattering calculation would make this option more user-friendly and allow more scenarios to be evaluated with limited time and computer resources. Of the three extensions above it is thus given highest priority.

2.1.2 Scattering by oriented particles

One of the uncertainties in estimating the global radiative impact of cirrus clouds is the orientation of the ice particles in space. A cirrus cloud composed of horizontally oriented ice crystals has a larger plane albedo than a cirrus cloud composed of randomly oriented particles. A good summary of the state of knowledge about prefered orientation of ice crystals (remote sensing observations as well as theoretical and laboratory studies) is given in the introduction of Noel and Chepfer (2005). The assumption of randomly oriented particles allows great simplifications in the computation of crystal optical properties and radiative transfer. For this reason the assumption is made in almost all radiative transfer models including *libRadtran*.

In principle oriented particles could be included into the MYSTIC model if optical properties data is available. The major difficulty is the vast amount of memory that is required. For randomly oriented particles the scattering phase matrix depends only on the scattering angle, e.g. the angle between incoming and scattered directions. Moreover, the phase matrix has only 6 independent elements. In case of oriented particles the phase matrix depends on incoming and scattered direction, each of which is specified by a zenith and an azimuth angle. Therefore the phase matrix depends on 4 variables instead of only 1 as for randomly oriented particles. All 16 elements of the phase matrix are independent. The same is true for the extinction matrix, which in case of randomly oriented particles is diagonal and depends only on the scattering angle. The complexity of the optical properties for oriented particles makes it almost impossible to pre-calculate optical properties data and store it.

A way out of this problem would be to include a geometrical optics module into MYSTIC and to compute the optical properties online in the radiative transfer simulations. This approach would work for the visible spectral range where the geometrical optics approximation is valid. The optical properties would only be calculated for the specific directions and the individual calls to the geometrical optics module would probably be very fast. The geometrical optics module should be developed within the study.

For the thermal spectral region where the geometrical optics approximation is not valid other programs are needed to compute the optical properties, e.g. programs that use the T-matrix method. This method is probably too slow to compute optical properties online. Therefore there must be a possibility to use also pre-calculated data of optical properties. For this purpose we could only provide an interface to an existing tool, e.g. the freely available T-matrix codes by Mishchenko (`http://www.giss.nasa.gov/staff/mmishchenko/t_matrix.html`).

2.1.3 Polarized ground reflection for land surfaces

During the ESASLight project polarization has been included into the MYSTIC solver (Emde et al., 2009). The surface can be handled as a Lambertian reflector, for which all reflected light is unpolarized. For water surfaces a bidirectional polarized reflectance matrix (`http://www.giss.nasa.gov/staff/mmishchenko/brf/`) has been included which is based on the parameterization by Cox and Munk (1954) for the slope of the surface waves.

Bidirectional reflectance matrix parameterizations are not yet available but will become soon

(O. Haasekamp, personal communication). These new parameterizations could be included into MYSTIC.

2.1.4 Include effective variance in cloud specification

The scalar radiance that is reflected by or transmitted through the cloud can be described rather well by using two parameters to specify the cloud: the cloud optical thickness or the water content, and the effective particle size. Polarized radiances however are also sensitive to the width of the droplet/particle size distribution, or the effective variance.

So far it is not possible in *libRadtran* to specify the cloud effective radius independently from the width of the size distribution. A desirable extension for instance for MYSTIC would be the option to specify for each grid cell the water content, the effective radius, and the effective variance. Similarly for the 1D solvers it should be possible to specify effective variance profiles. Such an extension would require a major restructuring of the code.

A problem with this extension is that it is not possible to pre-calculate optical properties data for all combinations of effective radii and effective variances for the whole spectral range. Here the solution would be to store pre-calculated single scattering data (i.e. optical properties for single particles of various realistic sizes) and perform the averaging over the size distribution within *uvspec*. Again this is a major restructuring of *uvspec*.

2.1.5 Lidar and Radar simulator

Since the Lidar technique is an essential part of several coming and planned ESA missions (ADM/Aeolus, EarthCARE), the inclusion of Lidar in the *libRadtran* toolbox is highly desirable. The main purpose of doing that would be to include the effects of multiple scattering which is required because of the large footprint of the laser in the Earth's atmosphere. Accurate simulations of Lidar including higher orders of multiple scattering have so far only been done with Monte Carlo techniques, although the lidar geometry is one of the most demanding applications for Monte Carlo in atmospheric radiative transfer. This is easily illustrated by the fact that even in real life only a few photons reach the detector although the laser pulse includes many orders of magnitude more photons than a Monte Carlo model could trace within reasonable compulational time. Sophisticated variance reduction techniques are therefore required. We estimate the time to develop a reliable and bias-free lidar simulator to about 1 - 2 person years which might be highly desirable but probably beyond the scope of the follow-up ESASLight project. The same is true for a Radar simulator which, however, is complicated by the fact that coherent scattering might need to be considered.

2.1.6 Include new polarized 1D solver

Within the ESASLight study it has been recognized that the 1D polarized solver in *libRadtran* is quite inaccurate, mainly because it can not handle highly peaked phase matrices accurately. Several codes are available that include methods like second order intesity corrections (also implemented in the 1D scalar solver DISORT2). In the study by Kokhanovsky et al. (2009) several polarized radiative transfer codes (including MYSTIC) are compared, most of them agree very well even in the region of the forward scattering peak. The codes are briefly described in the paper, some of them are freely available. The models to come into consideration should be tested. The best model should be included as new solver into *libRadtran* provided that permission from the developer is given.

2.2 Task 2 - Generation of databases

2.2.1 Optical properties of aspherical particles (aerosols and ice clouds)

For the OPAC aerosols, the T-matrix method can be applied to compute the single scattering properties of aspherical aerosol particles. The T-matrix method is valid for moderate size parameters. The aspect ratio of the aerosols should be chosen to be realistic. In order to find out what are realistic assumptions a literature review is needed. Size distributions required to average the single scattering properties are specified in OPAC.

Using the methods by Yang et al. (2000, 2005) single scattering data has been recalculated recently for the shortwave spectral region (G. Hong, personnel communication). Whereas in previous calculations, only the extinction and scattering coefficients as well as the phase functions were computed, the current version includes the full phase matrices required for calculations with polarization. This data can be used to pre-calculate optical properties of ice clouds. In addition to the single scattering data appropriate size distributions are required. As described in 2.1.4 it might be useful to not fix the effective variance of the size distribution since there is a large variability in nature. If *uvspec* would be restructured in such a way that the averaging of the size distribution is done within the program, the data calculated by G. Hong includes everything required for the optical properties database for ice clouds. For the thermal region however the data is not yet available.

2.2.2 Model atmospheres and absorption and scattering properties for Mars, Venus and Titan

libRadtran has already been applied to other celestial bodies, in particular Mars and Titan (Adriani et al., 2006; McKeever et al., 2006). Although this is certainly feasible, application of *libRadtran* to planets other than Earth requires considerable efforts by the user in terms of providing absorption atmospheric profiles of the relevant species; implementing new absorbers and cross sections into the *libRadtran* source code; providing appropriate solar irradiance data considering the orbital parameters of the planet or moon; and considering all kinds of other peculiarities like Martian dust storms or the organic haze layer of Titan. For reasonable application, *libRadtran* needs to be extended specifically for each planet and it is suggested that *libRadtran* will be extended by all requirements of some target objects (e.g. Mars, Venus and Titan) and that standard atmospheric and surface properties will be provided, similar to the standard atmospheres and other data already available for Earth.

2.3 Task 3 - GUI improvements

During the current ESASLight study a first version of a Graphical User Interface (GUI) for *uvspec* has been implemented. The GUI is fully functional and includes the generation of input files, running of *uvspec* and plotting of results. However, a GUI is never finished and several points to be improved and/or extended are listed below in no specific order.

- The GUI currently is capable of plotting a subset of the radiative output provided by *uvspec*. It may be extended to allow for plotting of more output parameters, for example polradtran output and plotting of user specified output.
- Furthermore, plotting of input profiles of the neutral atmosphere, clouds and aerosol profiles may be added in addition to plotting of the extraterrestrial solar flux.
- It would also be beneficial to include plotting of the 3D cloud fields and other 2D information used by MYSTIC.
- The visualization of user documentation may be improved.
- If an option is activated and this option inhibits other options, these options should be "grey'ed". This requires rethinking/redesign of the general *uvspec* input structure and coding.
- The GUI may be extended to include some of the other *libRadtran* tools, such as *mie*.

Finally, for ESA type applications one might consider to extend the GUI to become a full satellite instrument simulator including instrument characteristics, orbit information, various atmospheric and surface models of interest, tools for adding noise to measurements, simulation of the measurements, tools for generation of retrieval algorithms, modules for data analysis and testing and verification of retrieval algorithms. This is obviously outside the scope of ESASLight, but something to be considered for the future.

2.4 Task 4 - Comprehensive test suite

libRadtran has been designed as a modular toolbox and hopefully many extensions will be included in the future. In order to make sure that the introduction of a new option has no side effects it is important to have a verification tool that is always used when new code is added to the package.

libRadtran already includes a script that runs examples (currently about 60) delivered with the package. The script compares the results with pre-calculated values and outputs the differences. Small differences are acceptable because of the numerical accuracy which results in slightly different results for different compilers or different processors. The testing of the examples is always done when new code is committed to *libRadtran*.

However, these 60 examples can not cover all possible combinations of input options. Currently *libRadtran* has about 250 input options which can be more or less arbitrarily combined. This yields millions of combinations and it is impossible to test all of them.

In addition to the example tests three test suites should be developed:

- Testsuite A should test the setup of optical properties. This should run relatively fast, because it does not require any expensive radiative transfer calculations. All of the tests defined in testsuite A should be run regularly, ideally each time, when new code is commited to the *libRadtran* package.
- Testsuite B should check the radiative transfer simulations. This will be an extremely extensive testsuite which should run continuously. There might be thousands of test cases for each solver. The order of the tests will be random to assure that, e.g., not only one solver is tested on one day. The setup of this test suite has been started in the ESASLight study.
- Testsuite C should generate random input files and run these input files with the development version and the latest stable release of *libRadtran*. The test should assure that the development version is consistent with the last stable *libRadtran* version.

2.5 Task 5 - Cleaning and restructuring of code

The current ESASLight study focused on adding various new features to the code, the major ones being polarization, Raman scattering, and a completely new and much more convenient way to provide scattering phase functions and phase matrices. This involved major changes to the code by different authors. The logical next step is a consolidation of all these changes, to eliminate bugs introduced and to make sure that all existing and new model options work together as expected. A major step towards this aim was the development of an extended test suite for *libRadtran* which allows to automatically test if options still work as they did before the changes. This test suite is far from being finished and needs to be extended considerably, see section 2.4. In order to keep the *libRadtran* toolbox an useful and extendable tool it is strongly recommended to clean up the code while at the same time not adding new options continuously.

2.6 Task 6 - Dissemination of *libRadtran*

2.6.1 Organize *libRadtran* workshop

Provided enough interest by *libRadtran* users it is suggested to organize a *libRadtran* workshop. While the manual certainly helps to get users started with *libRadtran* and while users experienced with radiative transfer should not have any difficulties running it, the average user with an average background in radiative transfer could greatly benefit from such a workshop. This is even more relevant for the three-dimensional MYSTIC Monte Carlo code which was not part of the free release previously and which adds a considerable amount of complexity. In our experience so far, users generally required help to get started with three-dimensional setups which cannot be provided by a written description alone.

The workshop would be split into two parts: An introductory part where usage and relevant features are explained by developers and experienced users; and a second part where specific problems of the users would be addressed with the help of several *libRadtran* experts. We envisage between 20 - 30 participants in a workshop which could be regularly held every two years.

2.6.2 Webpage

libRadtran and additional data can be downloaded from the webpage `www.libradtran.org`. This webpage needs continuous maintaining. Traditionally there is a new *libRadtran* release at the end of each year which needs to be put on the webpage along with the corresponding data packages. The webpage also includes a list of publications which have used *libRadtran*. This list is continuously updated. A user area has been added to the webpage where *libRadtran* users should contribute by adding their particular applications, and by sharing their experiences and tricks. So far there are unfortunately no external contributions. This means the promotion for the user area needs to be improved.

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