Towards a Generic Radiative Transfer Model for the Earth's Surface-Atmosphere System:
ESAS-Light, Contract No AO/1-5433/07/NL/HE

Executive summary

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1 Introduction

The aim of the ESASLight study was to develop a flexible radiative transfer toolbox for the Earth atmosphere-surface system in the solar and thermal spectral ranges. In particular, the toolbox should enable radiative transfer simulations that consider horizontal inhomogeneity, polarization, inelastic scattering, and spherical geometry. The *libRadtran* radiative transfer package, which already provided many of the required capabilities, was identified as the ideal starting point for this study. The toolbox shall strengthen ESA modeling capabilities for internal purposes (instrument and prototyping of inversion algorithms) and provide a set of standard radiative transfer tools for the development of ESA commissioned inversion schemes and calibration/validation activities. The long term objective of the project is to give actors in the field of remote sensing of planetary environments full access to a user friendly, well documented, and free of charge radiative transfer toolbox.

This report gives a short summary of the ESASLight project. Additional information can be found at `http://esaslight.libradtran.org/internal/Wiki/doku.php`.

2 The *libRadtran* radiative transfer toolbox

The *libRadtran* software package (Mayer and Kylling, 2005) is a suite of tools for radiative transfer calculations mainly for but not restricted to the Earth's atmosphere. It was found as an ideal starting point for the ESAS-Light study. *libRadtran* is freely available at `http://www.libradtran.org`. The *libRadtran* package may be used to calculate radiances, irradiances, actinic fluxes, and heating rates in the solar and the terrestrial part of the electromagnetic spectrum. It has been used for a variety of purposes (see the publication list at `http://www.libradtran.org/doku.php?id=publications`).

The design of *libRadtran* allows simple problems to be easily solved using default values and included data, hence making it suitable for educational purposes. At the same time the flexibility in how and what input may be specified makes it a powerful and versatile tool for research and development tasks. *libRadtran* has been verified in several model intercomparison campaigns, and validated by direct comparison with observations.

The *libRadtran* model was originally designed to calculate spectral irradiance and actinic flux in the ultraviolet and visible parts of the spectrum (Kylling, 1992) (initially the package was called *uvspec* and the radiative transfer tool still carries this name). Over the years *libRadtran* has undergone numerous extensions and improvements. Since about 2000, *libRadtran* has included the full solar and thermal spectrum, currently from 120 nm to 100 μm. *libRadtran* has been designed as a user-friendly tool which provides a variety of options to setup and modify an atmosphere with molecules, aerosol particles, water and ice clouds, and a reflecting surface as lower boundary. One of the most relevant features of *libRadtran* is that it includes not only one but a selection of about ten different RT solvers, fully transparent to the user, for different applications. The solvers include the widely-used DISORT code by Stamnes et al. (1988), a fast two-stream code (Kylling et al., 1995), the 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). The modular structure of *libRadtran* and the implementation in the standard C and Fortran77 programming languages makes it relatively easy to extend and further develop the package.

3 Model enhancements in the frame of the ESASLight project

The first task of the ESASLight study was to review which radiative transfer modelling capabilities are required for the analysis of current and future ESA missions and to identify the missing features in *libRadtran*. The main missing features identified were a polarization dependent 3D RT solver and a solver that considers inelastic scattering. New algorithms for these processes have been developed and implemented in *libRadtran* (Kylling et al., 2009). In addition, the treatment of water and ice cloud scattering has been completely redesigned and a large database of optical properties of water droplets and various ice particle shapes has been added. Aerosol modelling has been made more flexible, and a database of aerosol optical properties has been added. For the simulation of surface reflection more BRDF (Bi-directional Reflectance Distribution Function) models have been included. User friendly line-by-line tools to compute layer optical thicknesses which are required for high spectral resolution calculations using *libRadtran* have been provided. All new algorithms have been carefully validated by comparison against benchmark results and analytical solutions. In order to make *libRadtran* more user friendly the documentation has been completely rewritten. Various new examples, a chapter on the theoretical background of the radiative transfer solvers, and a "quick starting guide" have been added. Finally a first version of a graphical user interface has been developed which makes it easier for the user to generate input files, to run the RT solvers, and to visualize the results.

3.1 3D vector code (polarization)

The Monte Carlo solver MYSTIC has been extended to solve the vector radiative transfer equation in a three-dimensional atmosphere, and thus, to fully include all effects of polarization. Several methods to make the code accurate and at the same time efficient have been combined. The so-called "local estimate" method has been adapted for polarized radiative transfer and an importance sampling method is used to sample the photon direction after a scattering event. Highly sophisticated variance reduction methods have been implemented (Buras, publication in preparation) which allow a bias-free reduction of the computational time for cloudy atmospheres by orders of magnitude, where other codes require approximations like peak truncation or delta-scaling. In addition to implementing polarization-dependent scattering, all optical property databases had to be updated to store the scattering matrix rather than only the scalar scattering phase function.

Observations of polarized radiance may provide significantly more information about atmospheric constituents than unpolarized measurements, in particular about aerosol and cloud optical and microphysical properties. Polarization of atmospheric radiation is neglected by most radiative transfer models, although this neglection may give errors even in the unpolarized radiance of up to 10%.

3.2 Raman scattering

Molecules scatter solar radiation. Air density, temperature, molecular (re)-orientation, and kinetics, causing elastic and inelastic scattering, have primarily an effect on the spectral distribution of the scattered light. These phenomena split the scattering into several components: (i) an elastic scattering component termed the Gross line, (ii) the Brillouin lines which describe inelastic translational Raman scattering and (iii) inelastic rotational and rotational-vibrational Raman scattering. In the Earth's atmosphere the Gross and Brillouin lines may be combined into one elastic scattering component, the so-called Cabannes line. To explain filling-in of Fraunhofer lines it suffices to account for Rayleigh scattering and rotational Raman scattering. The classical Rayleigh scattering cross section includes attenuation of energy due to wavelength redistribution by rotational Raman scattering. To account for Raman scattering the wavelength redistribution must be accounted for in the emitted energy. A new solver "qdisort" that solves the RTE including Raman scattering has been developed, implemented in *libRadtran*, and extensively tested.

3.3 New optical properties for water and ice clouds and aerosol

The disort2 and MYSTIC solvers have been changed to directly use the tabulated phase function rather than the Legendre coefficients which allows much more efficient storage of optical properties, in particular the Mueller matrix required for polarization-dependent scattering. Improved databases of water and ice cloud optical properties were added to *libRadtran* with much higher spectral resolution than before.

A new set of aerosol optical properties has been generated. The refractive index of the aerosol particles and the size distributions were taken from the OPAC aerosol database (Hess et al., 1998) and the optical properties have been calculated with Mie theory assuming spherical particles. OPAC provides data for various aerosol types and offers typical aerosol type mixtures, for instance for continental polluted or desert conditions. This new addition to *libRadtran* makes it easy to specify arbitrary mixtures of basic aerosol types, e.g. water soluble aerosol, soot, or mineral dust.

3.4 Modelling of surface reflection

In addition to the already available BRDFs for water and land surfaces, the AMBRALS (Algorithm for Modeling [MODIS] Bidirectional Reflectance Anisotropies of the Land Surface) by Wanner et al. (1997) which allows a variety of kernel-driven semi-empirical BRDF models has been included in *libRadtran*. E.g. the MODIS BRDF product is provided in the AMBRALS format which is available at `http://www-modis.bu.edu/brdf/product.html` on a 1 km spatial resolution.

3.5 Graphical user interface

The various *libRadtran* tools have numerous options. This is especially true for the *uvspec* radiative transfer tool. To ease the writing of *uvspec* input files a graphical user interface (GUI) has been developed as part of the ESASLight project. The GUI may be used to create new or to modify existing input files. It furthermore interfaces several examples of *uvspec* input files thus making it easier for the user to get started. The GUI will run the *uvspec* model with the given input file and store the output to a user specified file. Finally, the GUI includes basic plotting capabilities of calculated radiation quantities.

3.6 Line-by-line tool

In order to perform high spectral resolution calculations using *libRadtran*, pre-calculated (layer) optical depths are required. A user friendly line-by-line tool which generates these input (data) as required for *libRadtran* has been provided by the Remote Sensing Technology Institute (IMF) at DLR. Based on atmospheric input parameters (pressure, temperature, and trace gas concentrations) and on spectroscopic data (line parameter databases), molecular absorption optical thicknesses are computed. The program utilizes efficient and accurate numerical methods for the computation of absorption cross sections (Schreier and Böttger, 2003; Schreier, 2006; Schreier and Kohlert, 2008).

4 Verfication and validation

The new algorithms have been carefully verified by comparison against benchmark results and analytical solutions. During the duration of ESAS-Light we took part in a model intercomparison study for polarized radiative transfer codes (Kokhanovsky et al., 2010) and in the SPARC CCMVAL Radiation intercomparison (publication in preparation) where *libRadtran* was considered the reference model. For Raman scattering as well as for polarization we found very good agreement with published results and conclude that the algorithms are correctly implemented.

5 Outlook

The development of *libRadtran* and MYSTIC is an ongoing project which will continue after the end of the ESAS-Light study. New active and passive observation methods continuously raise new demands to radiative transfer models and new processes and features will be included. ESAS-Light has given this development a great push, by concentrating the activities on some of the most important additions to be done which, however, are very demanding and would not have been possible without the ESAS-Light study.

In the course of the project, the next urgent steps were already identified and formulated in task 6 of the ESAS-Light study, "Recommendation for future evolution of libRadtran". In addition to a consolidation of the newly introduced features it includes some urgent improvements. Among others:

- develop a better k-distribution to replace the LOWTRAN band model
- introduce a different state-of-the-art 1D vector code
- improve user-friendliness of the GUI by considering the logical structure and interactions between input parameters
- re-organize structure and sections of the *libRadtran* code to enhance readability and extendability
- improve documentation of available input (atmospheric profiles, aerosol and cloud properties, ...)
- collect a set of examples simulating standard remote sensing instruments and geometries
- organize a workshop, to aid new users, educate existing users and to promote *libRadtran* in the scientific community.

We hope to be able to address these in the near future, possibly supported by an extension of the ESAS-Light study.

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