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

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WP4100: Verification plan

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1 Introduction

During the ESASLight study two completely new algorithms are developed: one is for the calculation of Raman scattering, the other is for the computation polarization using the Monte Carlo method. These new algorithms need to be validated carefully. This document presents a plan of how the validation will be performed. We have collected published results that can serve as benchmark for validation. Furthermore we have defined several test cases for solver intercomparisons as well as for physical consistency tests. We also propose to compare the simulations of polarized radiances to measurements.

In the last section of the report a rough plan for systematic testing of the whole *libRadtran* toolbox is presented. Three test suites should ensure that whenever new code is developed and committed to the software package this has no side-effects on other modules.

2 Raman scattering

Testing and verification of the Raman option include checking of the individual terms in the Raman source of the Raman radiative transfer equation, WP5100 report, Eqs. 34-35 , and comparison of final results with published results. Below a testing and verification plan is outlined.

2.1 Raman cross section

Some authors have published absolute rotational Raman scattering cross section relevant for atmospheric applications. They are listed in Table 1. These published results will be compared

Table 1: Published rotational Raman scattering cross sections.

Excitation wavelength	Comments	Reference
440 nm	T=250 K, N_2, O_2	Chance and Spurr (1997, Fig. 1)
310 nm	T=258 K, N_2, O_2	Sioris and Evans (1999, Fig. 1)

with the values from the cross section routines implemented in libRadtran.

2.2 Transmission

The transmission term $e^{-T(\tau_{\lambda_s})}$ in WP5100 report Eq. 35, will be plotted for a realistic atmospheric situation for various λ_s.

2.3 Single scattering albedo

Three different single scattering albedos are required to solve WP5100 report, Eqs. 34-35. The elastic single scattering albedo ω_λ^E is the same as used in the elastic calculation while $\omega_{\lambda_s}^R$ and $\omega_\lambda^{RL}(\tau_\lambda)$ represents the single scattering albedo for the Raman scattering gain and loss terms respectively. The elastic single scattering will be compared with earlier verified calculations excluding Raman scattering. No published results are available for $\omega_{\lambda_s}^R$ and $\omega_\lambda^{RL}(\tau_\lambda)$. The Raman gain and loss single scattering albedos will be calculated and their values assessed.

2.4 Photon conservation

Raman scattering conserves the number of photons. Hence, in a non-absorbing atmosphere the number of photons should be conserved. That the implementation of Raman scattering in *uvspec* conserves photons will be tested by using an artificial solar spectrum where all wavelengths have the same unit magnitude.

2.5 Single emission and absorption lines

To check the magnitude of the implemented Raman scattering, the effect on single emission and absorption lines will be evaluated.

2.6 Published results

A number of authors have published results related to Raman scattering in the atmosphere. Most of these works have been made in connection with ground based or satellite remote sensing applications. Below some of these results are described. The implementation of Raman scattering in *uvspec* will be compared against these results.

2.6.1 Filling-in factor

In the literature it is mostly the so-called filling-in factor (FI) that is reported in connection with Raman scattering in the atmosphere. Thus results from *uvspec* will be compared with published results of the (FI). However, several different definitions are used for the (FI) factor.

- The most common definition of (FI) is

$$FI_{Joiner}(\lambda) = \frac{I_{\text{inelastic}}(\lambda) - I_{\text{elastic}}(\lambda)}{I_{\text{elastic}}}. \quad (1)$$

  where $I_{elastic}(\lambda)$ is the elastic component of the radiation quantity of interest, and $I_{inelastic}$ is the same quantity including Raman scattering. It is noted that FI is frequently given in percent. This definition is used by for example Joiner et al. (1995); Vountas et al. (1998); van Deelen et al. (2005); Sioris and Evans (1999).

- A variation on this definition is used by Spurr et al. (2008).

$$FI_{Spurr}(\lambda) = 1 - \frac{I_{\text{elastic}}(\lambda)}{I_{\text{inelastic}}(\lambda)} = \frac{I_{\text{inelastic}}(\lambda)}{I_{\text{elastic}}(\lambda)} FI_{Joiner}(\lambda). \tag{2}$$

- A fractional FI factor is reported by Langford et al. (2007). It is defined as

$$FI_{Langford} = 1 - \frac{D}{D_0}, \tag{3}$$

  where the line depth is $D = I_2/(I_1 + I_2)$ (see Langford et al. (2007, Fig. 1b) for an explanation of I_1 and I_2). The D_0 line depth is taken from a direct sun spectrum.

- de Beek et al. (2001) reports the filling-in using Differential Optical Depths (DOD) which are defined as

$$DOD_{deBeek} = -\ln\left(\frac{I}{I_{ref}}\right) - P = -\ln\left(\frac{I_{\text{elastic}}}{I_{ref}}\right) - P - R \tag{4}$$

  where

$$R = \ln\left(\frac{I_{\text{inelastic}}}{I_{\text{elastic}}}\right) \tag{5}$$

  and P is a third degree polynomial that accounts for broadband features. For satellite situations $I_{ref} = I_0$ and for ground based locations clear sky spectra for noon time solar zenith angles are used.

Unless otherwise noted FI_{Joiner} will be reported.

2.6.2 Filling-in (FI) spectra

The most common illustration of the effect Raman scattering is in terms of FI spectra for a cloudless and aerosol free atmosphere. Examples of such spectra are listed in Table 2. The *uvspec* implementation of Raman scattering will be compared with these FI spectra. It is noted that several of the calculations presented in Table 2 use approximations that may effect the accuracy of the results. This include the number of the layers in the atmosphere and the number of angles used to represent the radiation field in the atmosphere.

2.6.3 Albedo, aersol, cloud and solar zenith angle effects

The effect of solar zenith angle have been reported for several wavelengths by several authors. Comparisons will be made with the results and conditions listed in Table 3.

Cloud effects on FI spectra have been reported by Spurr et al. (2008) and comparisons will be made with their results for the conditions listed in Table 4. Joiner et al. (1995, 2004); Vasilkov et al. (2008) have published results for FI using the Mixed Lambert-Equivalent Reflectivity

Table 2: Published cloudless filling-in spectra.

Wavelength	FWHM	Comments	Reference
300-340 nm[a]	1.1 nm	$\theta_0 = 45°$, z_{out}=TOA, $\mu = 1$, single-scattering	Joiner et al. (1995, Fig. 6)
355-400 nm		$\theta_0 = 87.5°$, z_{out}=TOA, $\mu = 1$, $A = 0.08$	Joiner et al. (1995, Fig. 11)
340-400 nm[b]	0.17 nm	$\theta_0 = 45°$, z_{out}=TOA, $\mu = 1$, $A = 0.1$	Joiner et al. (2004, Fig. 6)
310-410 nm[c]	22 cm^{-1}	$\theta_0 = 30°$, z_{out}=0, $\mu = -1$, $A = 0.22$	Sioris and Evans (1999, Fig. 6)
410-550 nm	22 cm^{-1}	$\theta_0 = 30°$, z_{out}=0, $\mu = -1$, $A = 0.22$	Sioris and Evans (1999, Fig. 7)
312-320 nm	22 cm^{-1}	$\theta_0 = 30°$, z_{out}=0, $\mu = -1$, $A = 0.22$	Sioris and Evans (1999, Fig. 8)
345-355 nm	0.45 nm	$\theta_0 = 61.42°$, $\phi = 71.72°$, z_{out}=TOA, $\cos^{-1}\mu = 57.59°$, $A = 0.049$	Spurr et al. (2008, Fig. 4)
315-335 nm	0.05 nm resolution	$\theta_0 = 45.0°$, z_{out}=TOA, $\mu = 1$, $A = 0.049$, Ozone column= 0 and 375 DU	Spurr et al. (2008, Fig. 6)
280-290 nm[d]	0.2 nm	$\theta_0 = 60°$, z_{out}=TOA, $\mu = \cos(30°)$, $\phi_0 = 10°$	van Deelen et al. (2005, Fig. 4)
320-330 nm	0.2 nm	$\theta_0 = 60°$, z_{out}=TOA, $\mu = \cos(30°)$, $\phi_0 = 10°$	van Deelen et al. (2005, Fig. 4)
390-400 nm	0.2 nm	$\theta_0 = 60°$, z_{out}=TOA, $\mu = \cos(30°)$, $\phi_0 = 10°$	van Deelen et al. (2005, Fig. 4)

[a]Triangular slit function, SSBUV resolution
[b]Triangular slit function, GOME resolution
[c]Triangular slit function
[d]Gaussian slit function

Table 3: Albedo and solar zenith angle effects on filling-in.

Wavelength	FWHM	Comments	Reference
393 nm[a]	1.1 nm	$\theta_0 = 0°\ldots 89°$, z_{out}=TOA, $\mu = 1$, $A = 0.08, 0.2, 0.95$	Joiner et al. (1995, Fig. 8)
393.4 nm[b]	0.17 nm	$A = 0.0, \ldots, 1.0$, z_{out}=TOA, $\mu = 1$, $\theta_0 = 0°, 30°, 45°, 60°, 70°, 77°, 84°, 88°$	Joiner et al. (2004, Fig. 2)
393.5, 358.5, 359.9 nm	1.1 nm	$\theta_0 = 0°\ldots 89°$, z_{out}=TOA, $\mu = 1$, $A = 0.08$	Joiner et al. (1995, Fig. 12)
285 nm	1.1 nm	$\theta_0 = 0°\ldots 89°$, z_{out}=TOA, $\mu = 1$, $A = 0.08$ $AOD = 0.0, 0.12, 0.42$	Joiner et al. (1995, Fig. 15)
396.969, 393.438, 352.612 nm	0.05 nm resolution	$\theta_0 = 20°\ldots 80°$, z_{out}=TOA, $\mu = -1$, $A = 0.1$	Spurr et al. (2008, Fig. 5)

[a]Triangular slit function, SSBUV resolution
[b]GOME resolution

Table 4: Aerosol and cloud effect on filling-in.

Wavelength	FWHM	Comments	Reference
344.1 nm[a]	0.33 nm	$\theta_0 = 0°...80°$, z_{out}=0.0, $\mu = -1$, $AOD = 0.0, 0.12, 0.42$	Langford et al. (2007, Fig. 5)
345-355 nm	0.05 nm resolution	$\theta_0 = 45°$, z_{out}=TOA, $\mu = -1$, $A = 0.05$ Cloud, 4-5 km, $\tau = 10$	Spurr et al. (2008, Fig. 3)
392-399 nm	0.108 nm resolution	$\theta_0 = 45°$, z_{out}=TOA, $\mu = -1$, $A = 0.05$ Cloud, 2-3 km, $\tau = 0.1, 1.0, 2.0, 5.0, 10.0$	Spurr et al. (2008, Fig. 7)

[a]Gaussian slit function

(MLER) concept to accout for clouds. Although *uvspec* may calculate results for similar conditions, we have chosen not to compare with these results here.

Aerosol effects have been reported by Langford et al. (2007) and *uvspec* will be compared with their results, Table 4.

Finally, Sioris and Evans (1999) have reported radiances with and without Raman scattering included. Comparisons will be made with these results for the conditions presented in Table 5.

Table 5: Miscellaneous results including rotational Raman Scattering.

Wavelength	Comments	Reference
313-314 nm	radiance, $\theta_0 = 30°$, z_{out}=0, $\mu = -1$, $A = 0.22$	Sioris and Evans (1999, Fig. 9)

2.6.4 Instrument response functions

In the UV-visible part of the spectrum the Raman effect is largely caused by inelastic scattering within approximately $\pm$2nm of the wavelength in question. Be however aware that the width of this interval depends on the wavelength and increases with wavelength. The rather narrow band effect of Raman scattering makes it highly sensitive to the spectral resolution of any instrument used to measure it. For example, Joiner et al. (2004) states that the atmospheric filling-in at OMI resolution (0.45-0.63 nm) is reduced by slightly less than 50% compared with GOME resolution (0.17 nm), for the cases they present. Also, simulations must be performed at high resolution and convolved with the appropriate instrument response function prior to comparisons with experiment. The full width at half maximum (FWHM) for the comparisons with published results planned here are provided in Tables 2-5.

3 Aerosol handling

For all aerosol types defined in OPAC optical properties have been generated using the Mie tool of the *libRadtran* toolbox. From OPAC the refractive indices and the aerosol size distributions were used as input. OPAC includes optical properties for scalar radiative transfer, e.g. phase

functions but no phase matrices. In order to validate whether we have used the OPAC data consistently with the original OPAC database of aerosol optical properties, we will compare single scattering albedo, extinction coefficient, asymmetry parameter and phase functions. Since the OPAC optical properties were also generated using a Mie program the scalar optical properties should be identical.

The next section deals with the verification of the implementation of polarization in the MYSTIC solver. In that section, solver intercomparisons are proposed, several test cases include OPAC aerosol types. Therefore these test cases are validations for the polarization as well as for aerosol handling. The same applies for a comparison to polarized radiance measurements in different aerosol conditions.

4 Polarization

4.1 Benchmark results

Even for a single plane-parallel layer including only molecules (pure Rayleigh scattering) there is no analytical solution for the polarized radiation field. A solution method has been derived by Chandrasekhar (1950). In this method the radiative transfer problem is expressed in terms of four pairs of the so-called X and Y functions, satisfying four pairs of simultaneous non-linear integral equations which can be solved by successive approximations. Such calculations were carried out in the 1950s independantly at the Watson Scientific Computing Laboratory in New York and at the Institute for Numerical Analysis of the National Bureau of Standards located at the University of California. From the values of the X and Y function Coulson et al. (1960) computed the Stokes parameters of radiation emerging in different directions from the top and from the bottom of the atmospheric layer for different sun elevations and different surface reflectivities. These computations were performed at the Western Data Processing Center at the University of California. In the 1950s the radiative transfer calculations required a huge effort, therefore Coulson et al. (1960) published a book including 548 pages of tabulated results of the computations.

Although we are now able to do such calculation within seconds on a simple PC, the tabulated results are very valuable for validation of a newly developed code. Tab. 6 shows seven test cases that we have defined for the verification.

All cases are performed with MYSTIC (new implementation of polarization) and with polradtran (1D vector code by Evans and Stephens (1991)). Both solvers are fully integrated in libRadtran. A simple test is to check that $U = 0$ in the solar pricipal plane which is obvious from symmetry arguments. This is checked in test case 1. In order to test whether the surface reflection has been implemented correctly, we have defined test case 4, which is for a very thin atmosphere and a large surface albedo. For all tests the Rayleigh depolarization as well as the molecular absorption will be switched off. The following solver-specific settings will be used:

- *MYSTIC:* Forward tracing mode, local estimate method switched on, 10 Mio photons, no Rayleigh depolarization, no molecular absorption

Case	τ	$\cos(\theta_0)$	$d\phi$	$\cos(\theta)$	A	z	Notes
1	0.15	0	0.0	(0.02, ..., 1.0)	0.0	b	principal plane $\Rightarrow$ U=0
2	0.15	0.4	(0.0, ..., 180,0)	0.64	0.0	b	almucantar plane
3	1.0	0.8	90.0	(0.02, ..., 1.0)	0.25	t	also shown in Evans and Stephens (1991)
4	0.02	0.92	(0.0, ..., 180,0)	0.4	0.8	t	test for surface reflection
5	0.25	0.92	(0.0, ..., 180,0)	0.02	0.25	b	very shallow viewing angle
6	0.25	0.92	(0.0, ..., 180,0)	0.4	0.25	b	low sun almucantar plane
7	0.25	0.92	60	(0.02, ..., 1.0)	0.25	b	low sun principal plane

Table 6: Test cases for comparison with tables by Coulson et al. (1960). Here τ is the optical thickness of the layer, θ_0 is the solar zenith angle, $d\phi$ is the azimuth angle between sun direction and viewing direction, θ is the viewing zenith angle, A is the surface albedo and z is the position (t - top of layer, b - bottom of layer).

- *polradtran:* 8 streams, 4 Fourier terms, 3 Stokes components

4.2 Test reciprocity principle for realistic atmospheres with molecules, aerosols, and clouds

MYSTIC can be run in different modes. In the "forward tracing" mode, photons are started at the top of the atmosphere with the solar zenith angle and the solar azimuth angle as initial direction and traced through the atmosphere where they may encounter multiple scattering processes. Finally they are counted at the sensor position. For the computation of radiances at a certain location it is more efficient to use the "backward tracing" mode. Here the photons are started at the sensor and traced backwards until they leave the atmosphere into the sun direction. The reciprocity principle, which von Helmholtz (1867) formulated for the first time, proves that the result is the same, no matter in which direction the photons travel through the atmosphere. We will check, whether it is fullfilled for three test cases:

1. standard midlatitude-summer atmosphere definded by Anderson et al. (1986) (pure Rayleigh scattering and molecular absorption)
2. standard midlatitude-summer atmosphere with additional "water soluble aerosol" as defined in OPAC (Hess et al., 1998)
3. standard midlatitude-summer atmosphere including a cloud with optical thickness 1 and an effective particle size of 10μm

These tests will be performed in spherical and in plane-parallel geometry.

4.3 Intercomparison between *libRadtran* radiative transfer solvers

In order to test the consistency of the various solvers that are available in libRadtran, we will perform polarized calculations using the Monte Carlo solver *MYSTIC* and the doubling-and-adding solver polradtran. The intensity results will also be compared with the well tested discrete-ordinate solver *DISORT2*.

Three aerosol types of the OPAC database will be used:

- water soluble (consists of various kinds of sulfates, nitrates, and other, also organic, water-soluble substances
- soot (absorbing black carbon)
- sea salt accumulated mode

These types have different optical properties: As in OPAC, optical properties of soot are calculated assuming many very small particles, the effective radius is about 0.05μm. Soot is the aerosol type with the smallest single scattering albedo (largest absorption coefficient). The water soluble aerosol consists of particles with an effective radius of about 0.15μm and the sea salt particles are the largest with an effective radius of about 1μm.

For each aerosol type the radiation field for two aerosol optical thicknesses will be calculated: 0.05 (very low aerosol content) and 0.5 (very high aerosol content).

4.4 Efficiency tests

To test the efficiency of the new code, MYSTIC will be run for different atmospheric conditions on a Intel Pentium processor with 2.8 GHz. The computational (CPU) times will be measured for scalar and vector calculations to see directly the difference. Of course the vector calculations should be slower than the scalar calculations because the code requires additional matrix multiplications and setting up the phase matrix instead of the phase function is more expensive. The same cases will also be computed using the solvers polradtran (vector and scalar) and DISORT (only scalar) on the same processor. CPU times can then directly be compared.

4.5 Comparison to measurements

Ground-based polarized radiance measurements have been conducted by Blumthaler et al. (2008). The measurements are performed at three wavelengths in the ultra-violet region of the spectrum and cover the solar principal plane as well as the almucantar plane. The Stokes components I, Q, and U are measured from which the degree of polarization can be derived. The measurements are performed in clear-sky conditions at several locations (Greece, New Zealand, Tenerife). The aerosol conditions are totally different: In Greece the measurements were performed in the polluted city Thessaloniki with high aerosol optical thickness. In Tenerifa the measurements were performed on the top of a mountain at 2367 m altitude where the aerosol

optical thickness is very small. These measurements are very well suited to validate the implementation of the OPAC database in libRadtran as well as the implementation of polarization in MYSTIC.

5 Test suites

The previous sections deal with the verification of the new algorithms that are implemented during the ESASLight study. Since further extensions are expected, 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*.

The 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.

We plan to include in addition to the example tests three test suites. The first one (testsuite A) tests 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.

The second one (testsuite B) should check the radiative transfer simulations. This will be an extremely extensive testsuite which should run continously. 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 third one (testsuite C) should generate random input files and run these input files with the develoment version and the latest stable release of *libRadtran*. The test should assure that the development version is consistent with the last stable *libRadtran* version.

In the course of the ESASLight study we will set up the first test suites. Setting up a “complete” test suite is a long term project and it will not be finished within ESASLight.

5.1 Grouping of options

In order to combine the options systematically for testsuite A we sort all options into different groups:

1. Molecules
2. Aerosols
3. Water clouds

4. Ice clouds
5. Surface
6. Radiative transfer solver
7. Miscellanous

Each of the groups 1-4 is devided into three sub-groups:

A Microphysics

B Parameterization

C Adjustments

When all options are grouped systematically it should be possible to generate input files for testsuite automatically. The tests should be set up for each of the groups 1–4 separately.

For testsuite B such a systematic setup is not feasible because there are too many combinations and the radiative transfer calculations require much more computation time. Here we need additional criteria like "commonly used combinations", which unfortunately can not be objective. Testsuite B can not cover all reasonable combinations but only the combinations that are frequently used.

5.2 The water clouds group (WC)

To demonstrate the systematic combination of options we have a closer look at the water clouds group (Tab. 7).

Microphysical data is required as input. This can be provided using one of the options `wc_file`, `wc_ipa`, or `wc_ipa_files`. `wc_cloudcover` makes only sense with `wc_file`, `wc_layer` and `wc_level` can be combined with all three input options. This makes 3+2+2=7 combinations for subgroup A.

In subgroup B we have 5 possibilities to choose the parameterisation (`wc_files` and 4 options for `wc_properties`). `wc_properties_interpolate` can be combined with only one of the parameterizations (mie), so we have alltogether 6 combinations for subgroup B.

Combination of all options in subgroups A and B gives 7·6=42 reasonable options to generate an input file.

Now all these inputs can optionally be modified using options in subgroup C. Scattering by water clouds can completely be switched off or optical properties can be modified. `wc_no_scattering` is independant of all other options. To modify the optical thickness one can choose `wc_set_tau` or `wc_set_tau550`. Similarly there are two options to modify the single scattering albedo and the asymmetry parameter respectively. So there are 3^3 ((option1, option2, no option)^3) combinations times 2 (`wc_no_scattering` set or not set), which makes 54 combinations. These apply for all cloud parameterizations except "mie". In

case of “mie” it does not make sense to specify the asymmetry parameter, then there are only $2 \cdot 3^2$=18 combinations.

In total there are $7 \cdot (4 \cdot 54 + 2 \cdot 18)$=1764 reasonable combinations to setup optical properties of water clouds.

Option name	Argument	Comments
A: Microphysics		
wc_cloudcover	[0–1]	-
wc_file	*filename*	file includes profiles of liquid water content and effective droplet radius
wc_ipa	*filename*	includes filename of a 3D cloud file
wc_ipa_files	*filename*	includes filenames of cloud profile data to be used for independant pixel calculation
wc_layer	-	input defined as layer property [default]
wc_level	-	input defined as level property
B: Parameterization		
wc_files	*filename*	Specify cloud extinction coefficient, single scattering albedo, and scattering phase function for each layer
wc_properties	4 possibilities	Choose parameterization. Possibilities are hu (Hu and Stamnes, 1993), echam4 (Roeckner et al., 1996), mie (pre-calculated tables), *filename* (user defined optical properties)
wc_properties_interpolate	-	needed for mie, if calculated wavelength not included in Mie table
C: Modifications		
wc_no_scattering	-	switch off water cloud scattering
wc_scale_gg	[0–1]	scale asymmetry parameter of Heney Greenstein phase function (works only with hu and echam4)
wc_scale_ssa	[0–1]	scale single scattering albedo
wc_set_gg	[-1–1]	set asymmetry parameter of Heney Greenstein phase function (works only with hu and echam4)
wc_set_ssa	[0–1]	set single scattering albedo
wc_set_tau	[0–∞]	set cloud optical thickness
wc_set_tau550	[0–∞]	set cloud optical thickness at 550 nm

Table 7: The option group *WC* for water clouds.

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