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Comparison of RTTOV and DISAMAR for clear sky and aerosol cases

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KNMI

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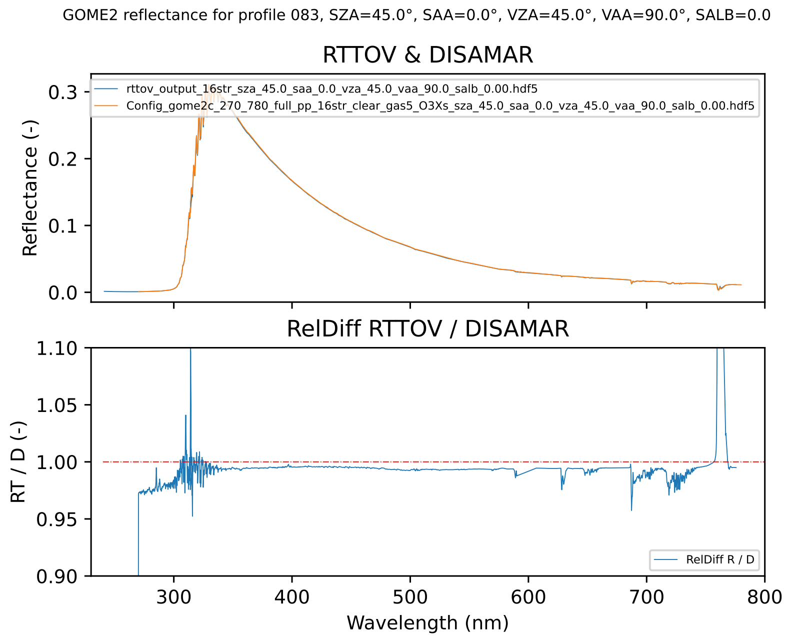
for clear sky and aerosol cases



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Chapter 1

Introduction

1.1 Motivation for this study

Satellite observations in the long wavelength parts of the spectrum (such as IR and microwave) have are regularly assimilated into forecasting systems for global weather predictions. Assimilating radiances in the UV and visible part of the spectrum has posed many challenges. The reason for this lies in the interactions of cloud, ozone and aerosol particles with radiation at those wavelengths as well as the often complex characteristics of the surface. These complications make it more difficult to develop 'observation operators', which convert model values into simulated satellite spectra.

For assimilation of atmospheric composition variables, the level-2 retrieval products are mostly used. This is the case for the Copernicus Atmosphere Monitoring Service (CAMS) at ECMWF, which develops and maintains 4D-Var assimilation and operational forecasts of trace gases, greenhouse gases and aerosols. While the L2 products used in the analysis are of very high quality [Inness et al., 2019], as new satellite instruments are being launched and new products developed and refined, it has become difficult to characterize the relative uncertainties and biases of the various Aerosol Optical Depth (AOD) and ozone products.

Due to these challenges, ECMWF has started exploratory work to use reflectances in the visible to characterize aerosol properties [Benedetti et al., 2020]. Using radiances directly in the forecasting model could be more useful, once implemented. The error characterization of radiances is more straightforward than that of L2 products and assimilation assumptions can be made all consistent (i.e., the same aerosol/ozone model is used from emissions to TOA radiances). Recent studies have also shown the potential of UV aerosol index assimilation [Zhang et al., 2021].

The use of UV information allows to constrain parameters other than AOD (for example single scattering albedo) and this helps with the characterization of absorbing aerosols such as black carbon. The interest in these types of aerosols is two-fold:

on the one hand they contribute to pollution and affect air quality levels, on the other they have a net radiative warming effect which can contribute to enhance green-house gases induced global warming. Moreover, long time series of observations from a range of satellite sensors with an almost global coverage are available from European and international space agencies, which can be exploited for reanalysis applications.

1.2 The objectives

The general high level objectives of the cooperation between parties in the project proposal were:

1. To start the exploitation of the RTTOV UV developments for potential operational applications and clarify user requirements for RTTOV UV, together with the developers. Questions to be answered:
   (a) Which users want what species, with prioritisation. For example:
      i. Aerosols in the UV, absorbing aerosols
      ii. Ozone profiles in the UV
   (b) Accuracy of the UV radiances
   (c) Is linear polarisation and/or multiple scattering needed?
   (d) Is rotational Raman scattering needed?
2. To benchmark the spectra generated by RTTOV in the UV against an established line-by-line RTM in the UV (DISAMAR, KNMI)
   (a) DISAMAR line-by-line radiances should be integrated over the spectral response functions of the sensor that is being simulated with RTTOV.
   (b) Benchmark cases: choice of suitable cases, e.g.: clear case, aerosol case, ozone case.
   (c) Lambertian surface in DISAMAR.
3. To start a collaboration between researchers involved in NWP and ACSAFs over common interests.
   (a) Hyperspectral retrievals
   (b) Atmospheric composition as input for NWP models, to improve e.g., circulation, atmospheric heating.
   (c) Surface characteristics at different wavelengths.

1.3 Mission deliverables

The deliverables were defined as follows:

1. Comparison of full radiative transfer radiance output in the UV of DISAMAR versus RTTOV, for the selected cases, with computation times involved.
2. Contribution to the definition of requirements for a full use of RTTOV UV for aerosol UV applications in collaboration with identified users.
3. Short report on work achieved during the AS.

1.4 Work plan

1. Make an inventory of what can be simulated with RTTOV and DISAMAR in the UV.
2. Define the cases for comparison.
3. Setting up the models with matching configuration
4. Running the models for the cases
5. Comparison of radiances
6. Conclusions

Requirements from users questionnaire for products in UV / UV aerosol index as first goal. This should be coordinated by NWP SAF with input and support from ECMWF and KNMI.

Chapter 2

DISAMAR and RTTOV

2.1 DISAMAR

DISAMAR (Determining Instrument Specifications and Analysing Methods for Atmospheric Retrieval) is a radiative transfer model developed to study instruments specifications and analyze retrieval algorithms for satellite instruments for the wavelength range from 270 to 2400 nm. DISAMAR contains a radiative transfer module to simulate radiance, irradiance, and sun-normalized radiance (or reflectance). It includes two forward simulation methods (Doubling-Adding method and Layer-Based Orders of Scattering (LABOS)) and three retrieval methods. The derivatives of the radiance or reflectance with respect to the retrieved parameters (also called weighting functions or Jacobians) are calculated using semi-analytical expressions. The atmosphere is assumed to be plane-parallel with an option for pseudo-spherical correction. Instrument features, such as signal-to-noise ratio, straylight, instrument spectral response function, and noise can be specified in DISAMAR.

DISAMAR includes multiple scattering, and options for polarization, rotational Raman scattering, various gas absorptions. Clouds and aerosols can be specified at pressure layers as scattering particles with a Henyey-Greenstein phase function or an expansion coefficient file of scattering phase function. The single scattering albedo and extinction coefficient of the clouds/aerosols layer are included in the expansion coefficient file. It is also possible to model a cloud or aerosol layer as a simple reflecting Lambertian surface. User can specify the atmospheric profile (pressure, temperature), gas mixing ratio profiles, cloud/aerosol layers etc. in a configuration file.

The surface is assumed to be a Lambertian reflector. Surface emission can be included to simulate sun-induced fluorescence. DISAMAR is a line-by-line model and the instrument spectral response function is used to convolve the spectrum at a high resolution grid to the instrument wavelength grid. The altitude grid in DISAMAR is calculated using temperature and pressure profiles assuming hydrostatic atmosphere. DISAMAR is focused on the accuracy but it is time consuming for the calculations. DISAMAR is open source software, available on Gitlab https://gitlab.com/KNMI-OSS/disamar. More details about DISAMAR are provided by De Haan et al. [2022].

In the UV, DISAMAR can simulate radiance and/or reflectance spectra with an atmosphere containing several trace gas species like O_3, NO_2, SO_2, BrO, formaldehyde, glyoxal, aerosol and cloud. For a simulation or retrieval, these need to be activated in the configuration when in use. For this study we used the trace gases listed in Table 2.1.

2.2 RTTOV

RTTOV is widely used in NWP models to simulate satellite measured radiances, brightness temperatures, and gradient of radiances with respect to state vector variables from ultraviolet to microwave wavelength ranges. RTTOV has TL/AD/K models to calculate the gradient of the forward model given an input profile. RTTOV uses parameterized optical thickness coefficient files for satellite instruments, so it is very fast. RTTOV computes transmittances by means of a linear regression in optical depth based on variables (predictors) from the input profiles. The coefficients of the optical depth regression are stored in an RTTOV coefficient file for a specific instrument. The RTTOV v13 predictors are valid up to SZA of 85°.

RTTOV can use a BRDF surface, various emissivity databases and aerosol climatologies. In this project, we use RTTOV to simulate GOME-2C spectra from 270 to 780 nm wavelength range, so we skip the description of RTTOV for the IR and MW wavelengths. In the UV/VIS wavelength range, the Rayleigh scattering is important. RTTOV can use single Rayleigh scattering with a BRDF surface. RTTOV can also use the DOM solver for multiple Rayleigh scattering or multiple scattering from clouds and aerosols. However, the DOM solver can only use a plane-parallel atmosphere and Lambertian surface. In the GOME-2C coefficient file, O_2, NO_2, H_2O and O_3 absorptions are taken into account. Rayleigh scattering is not included when making the coefficient file but calculated later during the simulations. The O_3 and H_2O profiles are variable, while the other gas profiles are fixed. The altitude grid is calculated from pressure and temperature profiles internally in RTTOV.

For the multiple Rayleigh scattering in the DOM solver, the depolarization factor is included in the calculation of the Rayleigh scattering cross section but not in the scattering phase function. The Rayleigh scattering cross section is taken from Eq. 8 with parameters in table 3 in Bucholtz [1995] and the phase function uses Eq. 11 in Bucholtz [1995] (also in Saunders et al. [2013] Eqs. 2.1.2–2.13).

There are no polarization and rotational Raman scattering in RTTOV. More details about RTTOV can be found in Saunders et al. [2018], Saunders et al. [2020] and Hocking et al. [2021].

In the UV, RTTOV can simulate spectra for those gases that are contained in the coefficients file. This is currently limited to O_3 (and water vapour). Clouds and aerosols can also be included in the simulation. In case other trace gas species need to be retrieved, then the coefficient file needs to be updated.

2.3 Differences and similarities between models

Each radiative transfer model has an orientation of the atmosphere (bottom-to-top, or vice versa), a definition of the orientation of the light paths (especially the definition of the (relative) azimuth angle), and maybe some conventions related to the calculation of the radiance or reflectance fields. In some cases some conversion / multiplication factors may be needed to bring the values from various models in correspondence with each other. For RTTOV and DISAMAR the main differences and similarities of the two models are given in Table 2.1.

Things to note from Table 2.1 are:

- Both atmospheres are set to plan-parallel; for the RTTOV DOM solver by default and for DISAMAR we turned off the spherical correction.
- The orientation of the azimuth angles are the same for both models (see section 2.4 for more detail)
- The wavelength grid of RTTOV was converted to nanometers (we may also have set RTTOV internally to output on a nanometer grid but for this study used the default).
- The reflectance of DISAMAR was calculated from the radiance / irradiance, with factors.
- The number of streams used was 16 in both models.
- The list of gases used in both models was brought in line with each other

2.4 Orientation of light paths

To confirm the orientation of the scattering and relative azimuth angle, we plotted the model results for various geometries.

In Figure 2.1 we show a series of RTTOV reflectances for an atmosphere with only Rayleigh scattering (surface albedo = 0.0). The SZA is fixed to 75 degrees and the VZA runs from 75 on a VAA of 0, through nadir, until 75 degrees with a VAA of 180. This spans a range of 180 to 30 degrees of scattering angle in the same plane, starting in an

Table 2.1: Model parameter and conversion factors

Model Parameter	RTTOV	DISAMAR
Horizontal atmosphere	Plan parallel	useCorrectionSphericalAtm = 0 ; 0: use plane-parallel atmosphere; 1: spherical correction for solar irradiance).
Vertical atmosphere	100 layers defined by 101 pressure levels	Pressure intervals divided by Gaussian division points
Backward scattering	SAA=0 & VAA=0	
Forward scattering	SAA=0 & VAA=180	
Wavelength to nm	1000 * 10000 / WaveNumbers	wavelength_radiance_band_1
Reflectance conversion	BtRefl (no conversion needed)	E / I_0 * π / cos ($\pi \cdot \theta_0$ / 180) E = earth_radiance_band_1 I_0 = solar_irradiance_band_1 θ_0 = solar zenith angle
NrOfStreams	DomNstreams = 16	nstreamsSim = 16
Polarization	Not available	Available, but not used
List of gases	RTTOV standard	O_2, O_3, NO_2, H_2O, O_2-O_2
O_3 cross sections	in RTTOV G2 coefficients	Derived from RTTOV
NO_2 cross sections	in RTTOV G2 coefficients	Origins: (in Vandaele et al., 1998)
H_2O cross sections	in RTTOV G2 coefficients	Hitran 2012
O_2 cross sections	in RTTOV G2 coefficients	Hitran 2012
O_2-O_2	in RTTOV G2 coefficients	Fally et al., 2020

orientation where the light is scattered backward, and ending in an orientation where light is scattered in a more forward direction.

Both RTTOV (Fig 2.1) and DISAMAR (not shown) provide the same pattern: the first line (SZA 75, VZA 75 and azimuth 0) has the strong backward Rayleigh scattering peak, which first reduces with increasing scattering angle and then increases again when the light is scattered more forward.

In Figure 2.2 we show the reflectance spectra of three viewing azimuth angles cases: backward (VAA = 0), at 90 degrees (VAA=180) where the scattering angle is exactly 90 degrees, and a case where the VAA is not in the same plane as nadir. The results are as expected, and agree with DISAMAR as well.

This is a confirmation that both RTTOV and DISAMAR have the same orientation of their light paths and that the implementation of Rayleigh scattering in both models is the same.

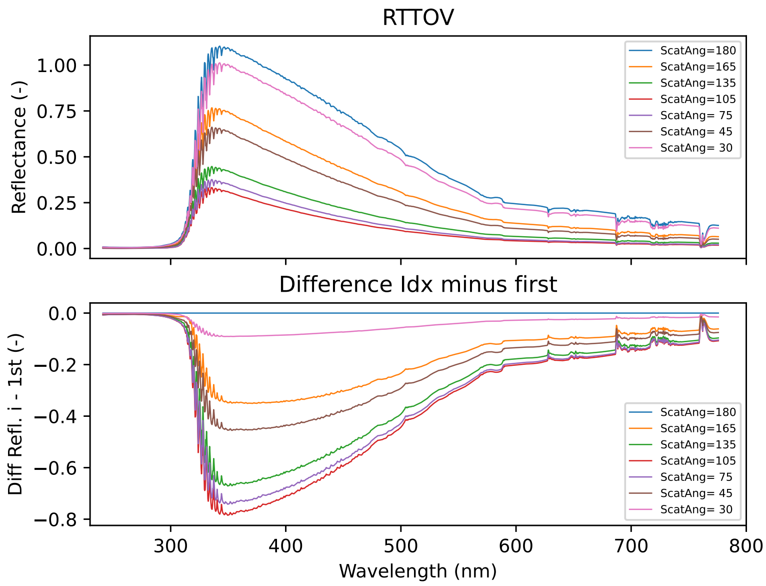

Figure 2.1: RTTOV reflectances (top) and difference w.r.t. first line for SZA 75 and various VZA in backward and forward scattering angle direction.

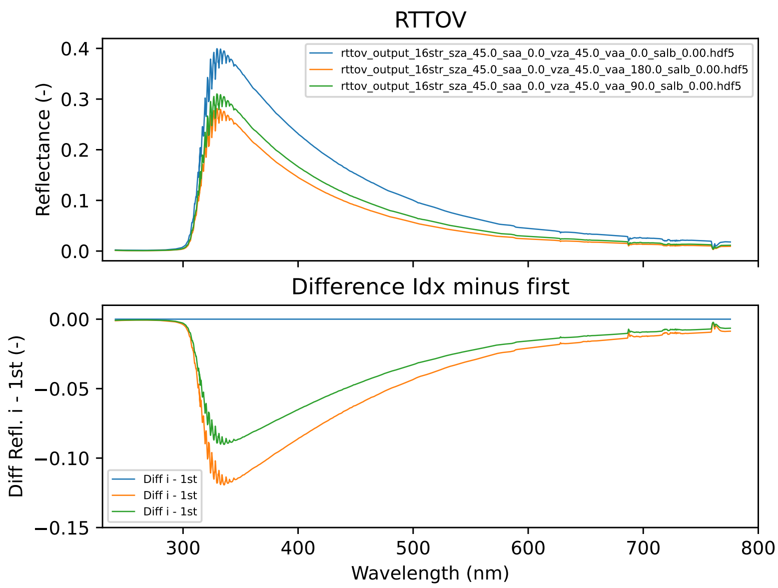

Figure 2.2: RTTOV reflectances (top) and difference w.r.t. first line for geometries with SZA 45 and VAA angles 0, 90 and 180 degrees.

Chapter 3

Methodology

3.1 Approach of the comparison of RTTOV and DISAMAR

We have compared RTTOV and DISAMAR simulations with multiple scattering for clear-sky scenes and aerosol scenes, respectively.

Both DISAMAR and RTTOV use the atmospheric profile 083 from the RTTOV data package, which include pressure, temperature, NO_2, H_2O, O_3, and O_2 profiles. In the comparison the RTTOV DOM solver is used because we want to use multiple Rayleigh scattering. Both the DOM solver and DISAMAR are set to use a plane-parallel atmosphere and a Lambertian surface.

3.2 Clear sky

For the clear-sky scenes, we used different surface albedo values, solar zenith angles and satellite viewing geometries to check a range of cases, listed in Table 3.1.

The Rayleigh scattering phase functions in RTTOV and DISAMAR are different. DISAMAR takes into account the molecular anistropy in the Rayleigh scattering phase function (see Eq. 12 in Bucholtz [1995]) which is more accurate than the Rayleigh scattering phase function used in RTTOV (see Eq. 11 in Bucholtz [1995]).

3.3 Aerosol

We did not use pre-defined optical properties for aerosols because the aerosol coefficient file for GOME-2C is not available yet. We created the same aerosol optical parameters in RTTOV and DISAMAR by ourselves.

Table 3.1: Model parameter ranges for clear sky cases

Model Parameter	Range
Solar Zenith Angle (deg)	0, 15, 30, 45, 60, 75, 85
Viewing Zenith Angle (deg)	0, 15, 30, 45, 60, 75, 85
Solar Azimuth Angle (deg)	0
Viewing Azimuth Angle (deg)	0, 90, 180
Surface albedo	0.0 and 0.8 shown in appendices; Data also available for 0.05 and 0.3

We used a strongly absorbing aerosol case from the ESA aerosol CCI project. The aerosol optical properties are calculated using the Mie code. The aerosol model has a log-normal distribution, with an effective radius of 0.142 micron, effective variance of 0.324 micron. The refractive index is 1.5 + 0.042i, same value from 320 to 400 nm. The phase function of the aerosols is shown in Fig. 3.1.

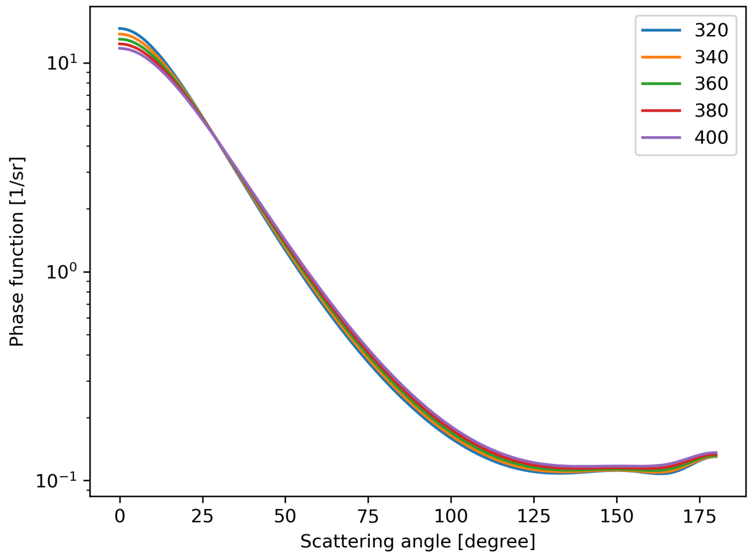

Figure 3.1: Phase function of the strongly absorbing aerosols at wavelengths from 320 to 400 nm, calculated using Mie codes. The refractive index is 1.5+0.042i for all wavelengths. The aerosol particles have a log-normal size distribution with effective radius of 0.142 micron and effective variance of 0.324 micron.

The same single scattering albedo (about 0.8), wavelength dependence of the AOT, and phase functions are used in DISAMAR and RTTOV. The aerosols are specified at one layer in the atmosphere between two pressure levels for three cases. The settings are given in Table 3.2.

In DISAMAR 60 Legendre polynomial expansion coefficients of the phase function are used. In RTTOV the Mie scattering phase function is used. The number of Legendre coefficient is 17 in RTTOV.

Table 3.2: Model parameter ranges for aerosol cases

Model Parameter	Range
Solar Zenith Angle (deg)	0, 30, 45, 60, 85
Viewing Zenith Angle (deg)	0, 30, 45, 60, 85
Solar Azimuth Angle (deg)	0
Viewing Azimuth Angle (deg)	0, 90, 180
Surface albedo	0.1
Optical thickness at 550 nm	0.0, 1.0, 2.0
Aerosol layer height	Pressure
Pressure 2km	802.3 – 777.8 (hPa)
Pressure 5km	535.2 – 515.7 (hPa)
Pressure 10km	272.9 – 260.0 (hPa)

Chapter 4

Results

We present DISAMAR and RTTOV simulated TOA reflectances at SZA = 45°, VZA = 45°, VAA = 90° as examples in this report. The SAA (Solar Azimuth Angle) is always kept fixed to 0° for all test cases because just varying the VAA (Viewing Azimuth Angle) leads to geometrically equivalent situations.

In order to keep the report concise and manageable, the bulk of the figures for all the clear sky and aerosol cases are provided as separate files. Please see Chapter 6 for a list of these appendices.

4.1 Clear-sky scenes

Figure 4.1 shows the RTTOV and DISAMAR simulated TOA reflectances for GOME-2C at SZA=45°, VZA=45°, VAA=0°. Surface albedo is 0. We can see that RTTOV and DISAMAR simulated reflectances have good agreement, the ratio of these two spectra is mostly within 1%, except for at the wavelengths with strong absorption of ozone below 300 nm, H2O close to 720 nm, and O2 close to 760 nm. Figure 4.2 is similar to Figure 4.1 but here the surface albedo is 0.8.

In the case with an albedo of 0.0, the light at TOA is caused purely by Rayleigh scattering, while for the case with an albedo of 0.8 the additional light reflected by the surface dominates and reduces the relative difference between the two models to practically zero (outside of the strongly absorbing bands).

There is an difference in the reflectances simulated by DISAMAR and RTTOV. The difference is mainly caused by the Rayleigh scattering phase function [Bucholtz, 1995].

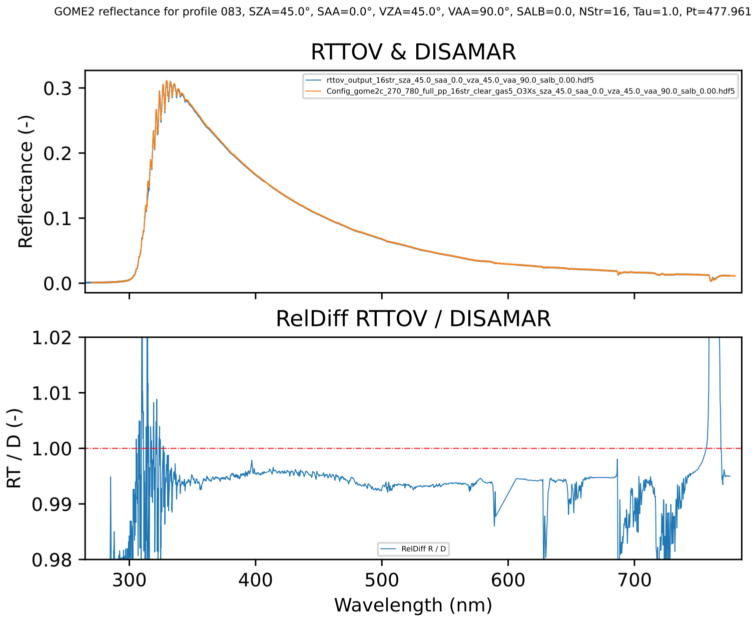

Figure 4.1: RTTOV and DISAMAR simulated TOA reflectances for a clear-sky scene at SZA = 45°, VZA = 45°, VAA = 90°, surface albedo = 0.0. The bottom plot contains the RTTOV / DISAMAR ratio.

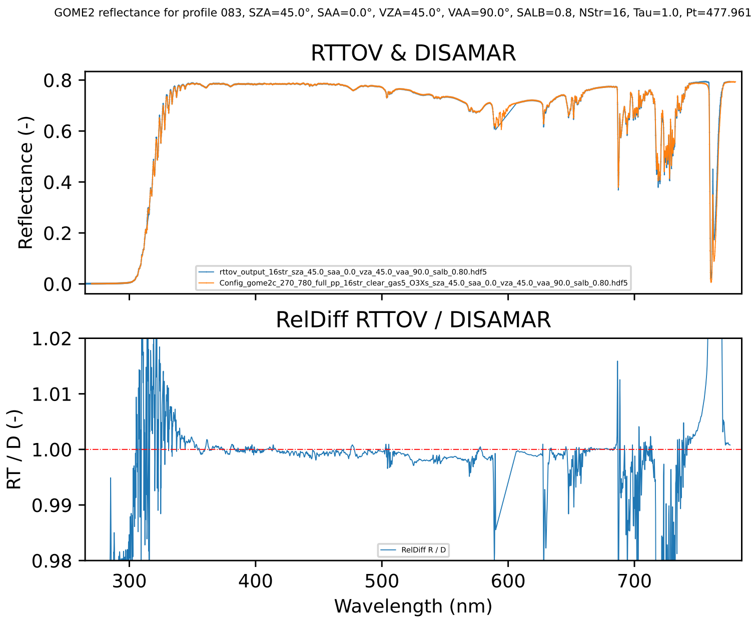

Figure 4.2: RTTOV and DISAMAR simulated TOA reflectances for a clear-sky scene at SZA = 45°, VZA = 45°, VAA = 90°, surface albedo = 0.8. The bottom plot contains the RTTOV / DISAMAR ratio.

4.2 Disabled depolarisation in DISAMAR

In the pure Rayleigh atmosphere cases of the previous section, there are varying differences for different geometries, usually running between $\pm$ 1 – 2%, depending on wavelength and geometry. The largest differences often occur with low SZA and/or low VZA with a lot of forward scattering.

DISAMAR includes a depolarisation factor of dry air and RTTOV does not, which could (in part) be the cause for the differences mentioned above. In order to test that hypothesis we removed this depolarization term in the DISAMAR Rayleigh scattering phase function, so that its Rayleigh scattering phase function is the same in DISAMAR and RTTOV.

We ran the same cases as above (in section 4.1), with the modified Rayleigh scattering phase function in DISAMAR. Figures 4.3 – 4.4 show the comparison of these cases.

The agreement between the models is clearly better: now usually within 0.5% (outside absorbing bands), and this confirms our hypothesis that the depolarization of air was one of the causes of the remaining differences.

While differences between DISAMAR and RTTOV varied with the geometry (zenith and azimuth angles) for the regular clear sky cases, this feature disappeared when using the same Rayleigh scattering phase function (i.e.: no depol for DISAMAR). The difference between the models seems to be the same across almost all geometries.

The remaining 0.2-0.5% differences outside the gas absorption bands may come from the Rayleigh scattering cross section, interpolation of temperature and pressure profiles, or RTTOV optical thickness coefficients.

The Rayleigh scattering cross section from RTTOV is about 0.1-0.3% lower than the Rayleigh scattering cross section used in DISAMAR in the UV wavelength range. Using more vertical layers in DISAMAR will change the reflectances of less than 0.1% below 300 nm but the impact may be 0.2 % at 320 nm for albedo of 0.8. The interpolation method of linear or cubic spline for the O_3 profile, has about 0.2% difference at 305 nm, causing a larger reflectance in a linear interpolation. We used cubic spline interpolation in all simulations.

The RTTOV GOME-2C coefficients are trained based on LBLRTM 12.8. The differences between RTTOV and LBLRTM 12.8 simulated reflectances for GOME-2C are available on the NWF-SAF website (https://nwp-saf.eumetsat.int/site/software/rttov/download/coefficients/comparison-with-lbl-simulations/#visir_lbl_comp_v13pred). The mean difference of the reflectances are almost zero but the standard deviation of differences is up to 0.001 at the O_3, H_2O, and O_2 absorption lines. This feature is similar to the reflectance differences between RTTOV and DISAMAR.

We would like to recommend to NWP-SAF to consider implementing the depolarisation factor of air into RTTOV.

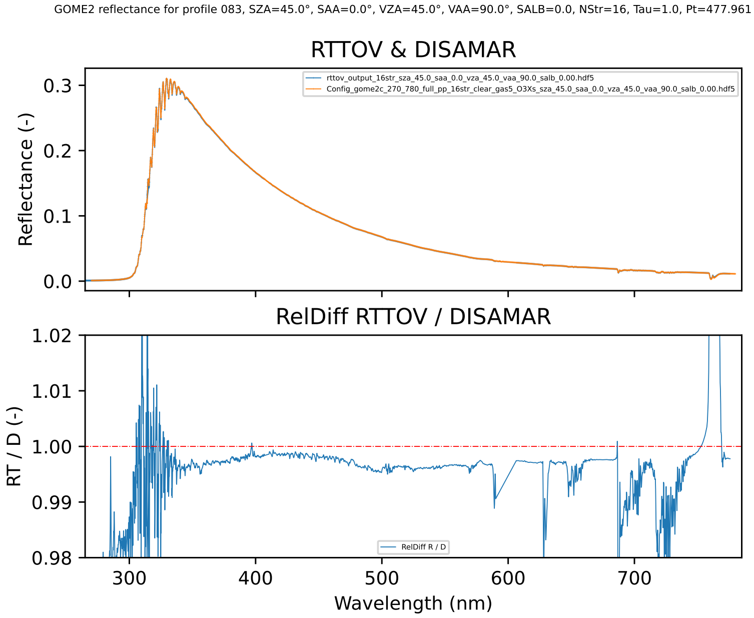

Figure 4.3: RTTOV and DISAMAR simulated TOA reflectances for a clear-sky scene at SZA = 45°, VZA = 45°, VAA = 90°, surface albedo = 0.0. No depolarization in Rayleigh scattering phase function.

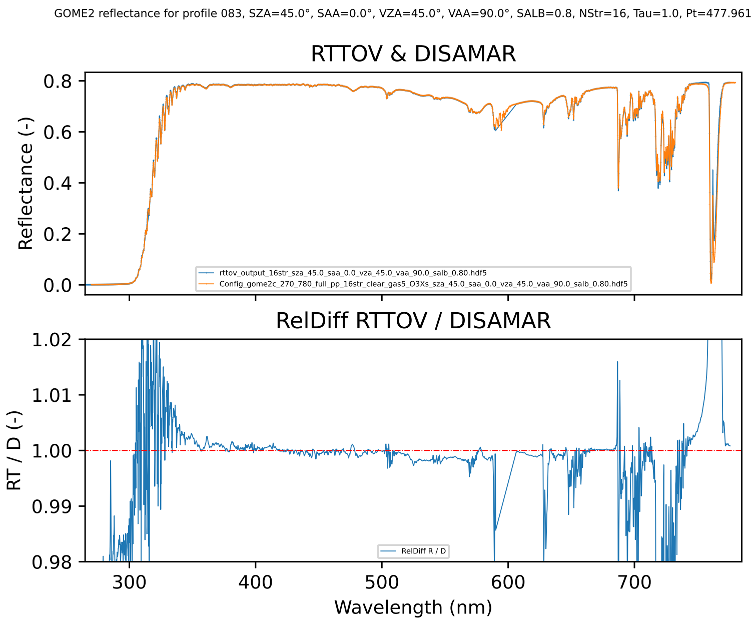

Figure 4.4: RTTOV and DISAMAR simulated TOA reflectances for a clear-sky scene at SZA = 45°, VZA = 45°, VAA = 90°, surface albedo = 0.8. No depolarization in Rayleigh scattering phase function.

4.3 Ozone and O_2 A-band

In this section we zoom in a little to spectral ranges of interest: the ozone absorption band and the O_2 A-Band, because both show varying differences with wavelength.

4.3.1 Ozone

We used the same O_3 cross section (provided by MF) but there are still some small differences. For the spectral range of 320 – 330 nm, the position of the ozone absorption peaks and troughs seems to be the same, but in the troughs the agreement of the reflectance between the models is better than in the peaks. For example: the peak at 321 nm is 1-2% off at a reflectance of 0.35, but the trough at 328 nm seems to agree (close to 0%) at a reflectance value of 0.35.

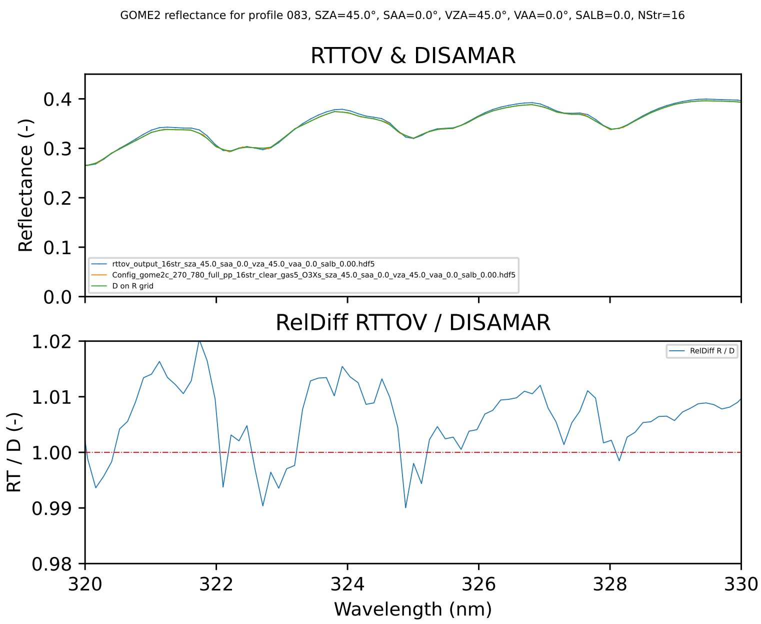

Figure 4.5: RTTOV and DISAMAR simulated TOA reflectances for a clear-sky scene at SZA = 45°, VZA = 45°, VAA = 0°, surface albedo = 0.0. Zoom of O_3 band.

4.3.2 O_2 A-Band

The differences between RTTOV and DISAMAR simulated reflectance is about 2 – 30% at the deep absorption band close to 761 nm. We think this is due to the O_2 optical thickness coefficients in RTTOV. RTTOV v13.1 coefficients are trained using LBLRTM v12.8 where the AER spectral database v3.5 based on updated HITRAN2012 and the continuum MT-CKD 3.2 . In DISAMAR, the O_2 line absorption parameters are also from

HITRAN 2012. As discussed in section 4.2, RTTOV and LBLRTM has relatively larger differences at the O_2 A band. It is consistent with our findings.

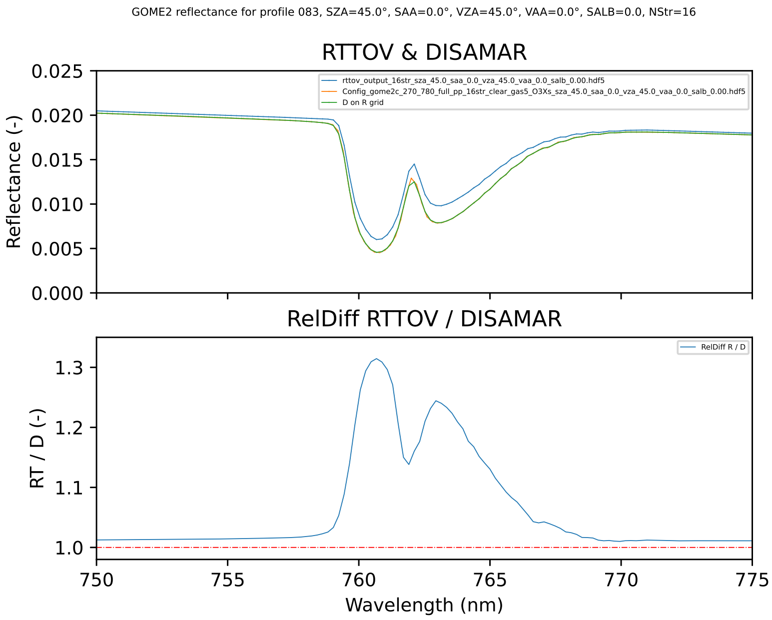

Figure 4.6: RTTOV and DISAMAR simulated TOA reflectances for a clear-sky scene at SZA = 45°, VZA = 45°, VAA = 0°, surface albedo = 0.0. Zoom of O_2 absorption band.

4.4 Aerosol scenes

For the aerosol cases we limit the spectral range to 330–390nm, because the phase function and scattering properties of the aerosol were only defined over this region. In all aerosol test cases, the surface albedo value is fixed to 0.1.

In this section we show the figures with AOT = 1 at three pressures around 2, 5 and 10 km altitude (see Figs. 4.8 – 4.10). The clear-sky scene with AOT = 0 is also shown in Fig. 4.7 for comparison.

The results, the simulated spectra RTTOV and DISAMAR, are in good agreement: within 1%. This is to be expected, because we use the same aerosol optical properties and phase function which was externally prescribed. However, the number of Legendre polynomial coefficients is different: 60 in DISAMAR, 17 in RTTOV but this seems to make almost no differences for these aerosol cases.

For the AOT = 0 scene, the offset between DISAMAR and RTTOV simulated reflectances is caused (in part) by Rayleigh scattering phase function.

The agreement between models is better for AOT = 1 than AOT = 0 because the contribution of Rayleigh scattering is relatively small when there are aerosols. The strongly absorbing aerosols absorb light, and reduce the amount of Rayleigh scattering below it. This effect is larger when the aerosol layer is at higher altitude (there is a lower reflectance at TOA with an aerosol layer at higher altitude).

The difference is larger than 1% when SZA = 85° and VZA = 85° for scattering in the forward direction. The single-scattered contribution (TMS correction) is computed by interpolating the phase function, rather than reconstructing the phase function from a large number of Legendre coefficients (as is done in DISORT, for example), so a higher number of streams would not make a difference for RTTOV.

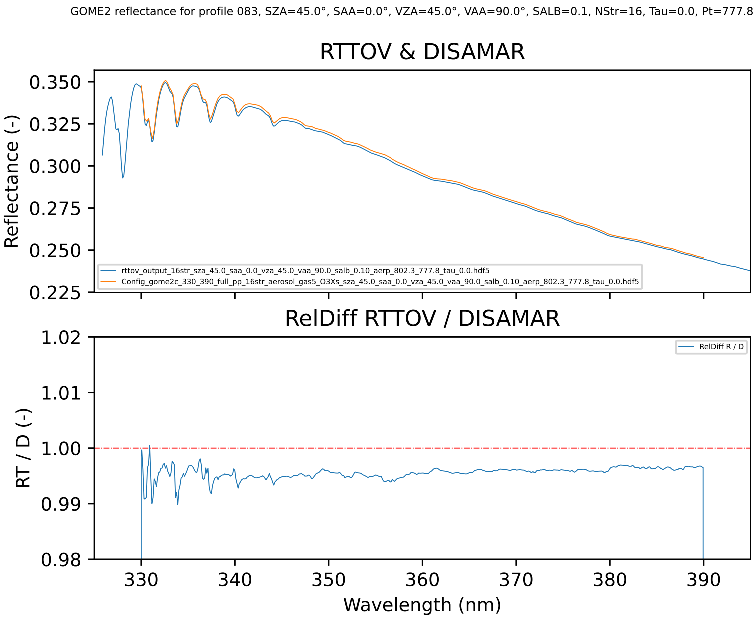

Figure 4.7: RTTOV and DISAMAR simulated TOA reflectances for clear-sky scene at SZA = 45°, VZA = 45°, VAA = 90°, surface albedo = 0.1. AOT = 0.0.

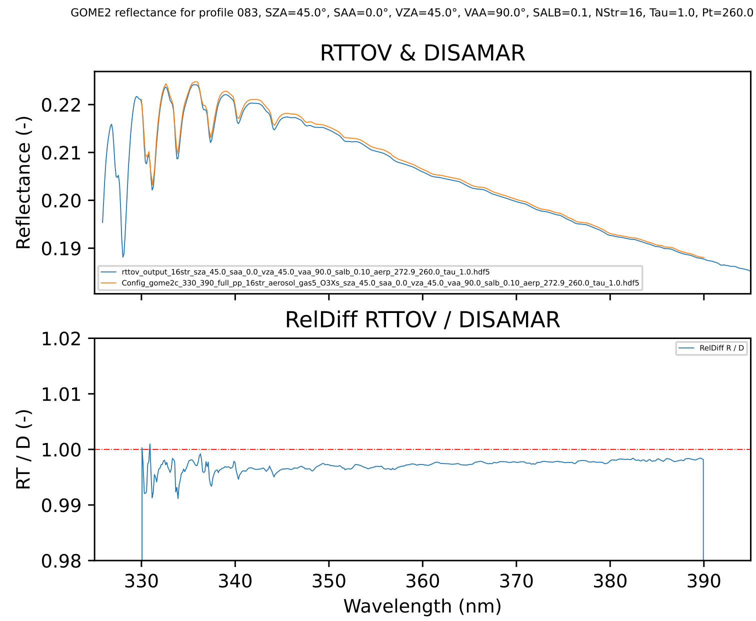

Figure 4.8: RTTOV and DISAMAR simulated TOA reflectances for an aerosol scene at SZA = 45°, VZA = 45°, VAA = 90°, surface albedo = 0.1. AOT = 1.0. A single aerosol layer is at 272.9 to 260.0 hPa.

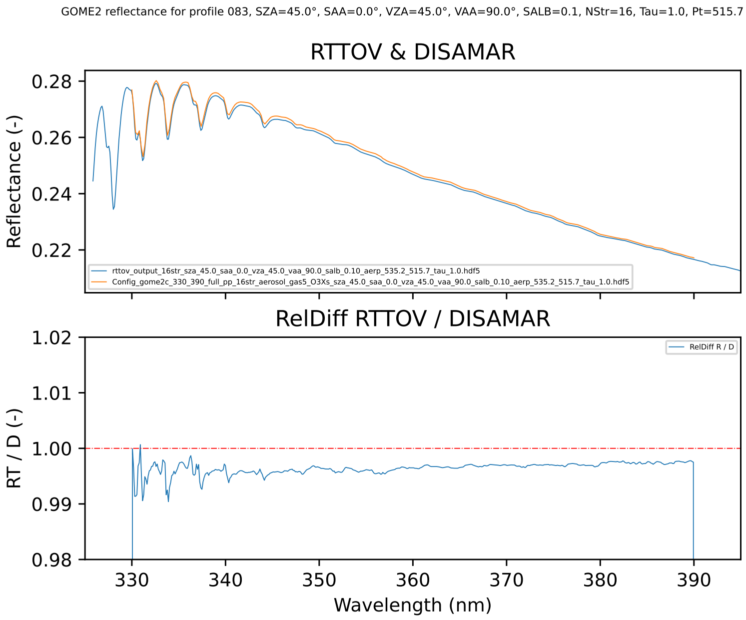

Figure 4.9: RTTOV and DISAMAR simulated TOA reflectances for a clear-sky scene at SZA = 45°, VZA = 45°, VAA = 90°, surface albedo = 0.1. AOT = 1.0. A single aerosol layer is at 535.2 to 515.7 hPa.

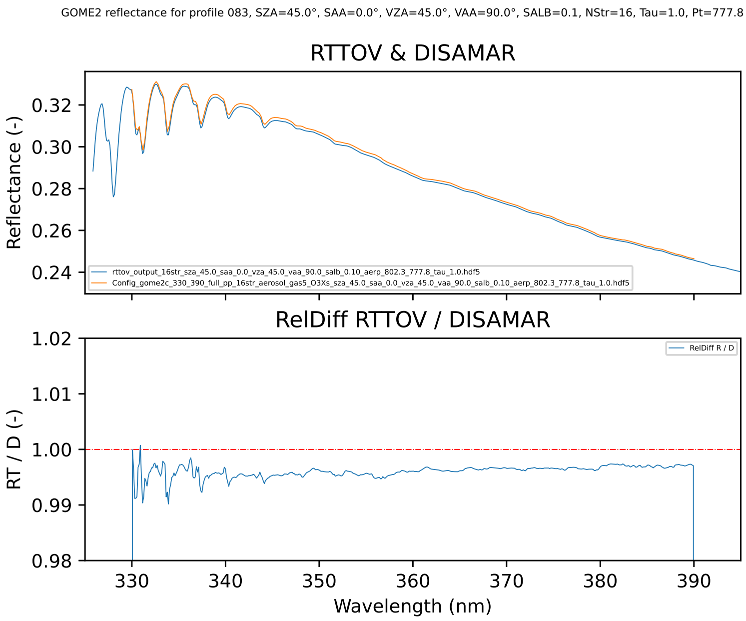

Figure 4.10: RTTOV and DISAMAR simulated TOA reflectances for an aerosol scene at SZA = 45°, VZA = 45°, VAA = 90°, surface albedo = 0.1. AOT = 1.0. A single aerosol layer is at 802.5 to 777.8 hPa.

4.5 Computation times

The calculations of both RTTOV and DISAMAR at KNMI were done on a set of workstations, not all completely free of other tasks, so the timing of the runs varies a little bit. In general, the computation times for the models can be seen in Table 4.1.

The computation of RTTOV (with its pre-convolved instrument coefficients) is fast compared to the line-by-line calculations of DISAMAR. Especially when the spectral range is wide, then DISAMAR is considerably slower than RTTOV.

Table 4.1: Computation time for the models

Model	Case	Run time
RTTOV	Clear sky (270 – 780nm)	$\approx$ 6 – 7s
DISAMAR	Clear sky (270 – 780nm)	$\approx$ 35 – 37m
RTTOV	Aerosol (330 – 390 nm)	$\approx$ 6 – 7s
DISAMAR	Aerosol (330 – 390 nm)	$\approx$ 1m

Chapter 5

Conclusions and outlook

5.1 Conclusions and outlook

We have compared RTTOV simulated TOA reflectances for GOME-2C with DISAMAR simulations for clear-sky and aerosol scenes. The differences between RTTOV and DISAMAR simulations are mostly with 1-2 % except for at wavelengths with strong gas absorptions where the reflectances are too low. These differences are comparable to the values provided in the RTTOV validation report.

In the comparison we provided the same input parameters to both models as best as possible, but DISAMARs radiative transfer calculation uses a Gaussian altitude grid internally onto which it interpolates the prescribed input temperature and pressure profiles coming from profile 083 from the RTTOV data package. The wavelength grid of RTTOV and DISAMAR is also different. RTTOV trained the gas absorption coefficient file at the GOME-2C wavelength grid. DISAMAR uses a high resolution wavelength grid, then convolves that HR spectrum with the GOME-2C ISRF and creates output at a wavelength interval of 0.2 nm. This creates some small differences for the O_3 and H_2O absorptions. Also, because RTTOV uses optical thickness coefficient files instead of raw absorption cross sections like DISAMAR, this leads to small changes in the actual gas absorption / optical thickness of the atmosphere.

In general, spectra from RTTOV (using its DOM solver) and DISAMAR are in good agreement in the UV and visible wavelength range for multiple scattering in clear-sky and aerosol scenes. The results may be different if we use other solvers (RTTOV with coefficient files, MFASIS).

The AD/TL/K are calculated in RTTOV have not been compared to DISAMAR. Given that these parameters are also important for the data assimilation and retrievals, it would be worthwhile to compare these in the future.

Polarization is not implemented in RTTOV yet so we have no comparison here. The difference with and without polarization depends on solar and viewing geometry and wavelength. At 320 nm, dark surface, the relative difference at SZA = 70°, VZA = 20°, RAA = 180° is about 9 – 10%, while the difference is less than 1% below 300 nm [De Haan, 2012].

Although the RTTOV and DISAMAR simulations are similar but they miss Raman scattering features that are present in real observations (like GOME-2 spectra). Raman scattering can also be compared with DISAMAR when it is has become available in RTTOV.

The comparison is performed for a Lambertian surface because DISAMAR has no option for BRDF surface yet. This can be implemented in the future.

The authors would like to recommend to the NWPSAF team that they include depolarisation of air in a future version of RTTOV, as this seems to be a relatively inexpensive calculation which would bring the model closer to known physics.

Depending on the accuracy requirement of the application, RTTOV can be a good and consistent RTM to simulate spectra for ozone and aerosol in the UV part of the spectrum, assuming that the neglection of polarisation is corrected for in the future.

5.2 Notes from the online meeting (14/sept/2022)

The following notes were made during the discussion of the project team during the online meeting at the end of the project.

- This was one of the first times that RTTOV was compared to other (line by line) models in the UV, and the agreement is quite good. However, the agreement between RTTOV and DISAMAR is only good in the hypothetical case that polarization can be neglected in multiple scattering. This is not the case for real world radiances (see below).

- The increasing difference in below 300nm was discussed, and a suggestion was made to check whether the models actually go up to 0.001 hPa, because from earlier experience with GOME-2 below 300nm it was demonstrated that cutting the atmosphere at 0.1 hPa creates a 10% difference in the radiance below 300nm. There is still air that causes Rayleigh at that altitude.

- The larger deviation in the O2-A band also needs to be investigated more. Oxygen is a strong absorber in this spectral region and that may not be quite accurately modelled in RTTOV. The predictors have not been tested in this spectral region. It would be good to investigate that further, so that RTTOV can be used for cloud work.

- For the future, it would be nice to use an actual aerosol profile to do the comparison (spanning multiple layers), and calculate an equivalent of the UV Absorbing

Aerosol Index. The NWP-SAF has the aerosol properties that are used in the CAMS model.

- A short discussion was held on the need of a surface albedo value for forward model AAI calculations based on CAMS/IFS atmospheric input. Land in the UV is quite dark, but water bodies can be brighter (up to 10%). It is probably OK to just assume a value, but it needs to be tested. If surface albedo values below 400nm are needed, one can look at the GOME-2 DLER or Tropomi DLER that may go down to 335nm.

- In the spectral range from 300nm to 500nm polarisation is becoming important for higher order scattering calculations. KNMI has a lookup table approach for correcting polarisation in models, depending on geometry, surface albedo and ozone. Maybe the albedo can be used as a proxy for AOD.

- Raman scattering also affects the peaks and valleys of the spectrum, with stronger absorbers. KNMI's experience is that this would likely double the calculation times, even with some kind of parameterisation.

- For the purpose of calculating the AAI, we don't think that Raman is of much influence because the spectrum (e.g.: around 340 and 380 nm) is usually averaged over a 1nm wide section and details of Raman are then averaged out.

- After the report is finished, maybe a short item can be made for the ECMWF and/or NWP-SAF newsletter.

- The (extended) project team was happy with the results so far and are looking forward to working together again in the future, on writing a paper and comparing the models again when new developments have been implemented in RTTOV.

Chapter 6

List of appendices and data packages

Appendices:

- Appendix A: Plots of the Clear Sky cases
- Appendix B: Plots of the Clear Sky cases, with disabled depolarisation in DISAMAR Rayleigh scattering phase function
- Appendix C: Plots of the Aerosol cases

Data packages:

- Data package A: output data of RTTOV and DISAMAR used for Appendices A
- Data package B: output data of RTTOV and DISAMAR used for Appendices B
- Data package C: output data of RTTOV and DISAMAR used for Appendices C

Scripts and other files:

- Example configuration file for DISAMAR for Clear Sky and Aerosol case, to be used with the Open Source version of DISAMAR available at: https://gitlab.com/KNMI-OSS/disamar
- Scripts used to run RTTOV to generate the clear sky and aerosol cases in this study
- Phase function used in both RTTOV and DISAMAR for the aerosol cases.

Chapter 7

List of acronyms

AAI	Absorbing Aerosol Index
ATBD	Algorithm Theoretical Baseline Document
BRDF	Bidirectional Reflectance Distribution Function
ECMWF	European Centre for Medium-Range Weather Forecast
ESA	European Space Agency
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
FOV	Field-of-View
GOME	Global Ozone Monitoring Experiment
HDF	Hierarchical Data Format
HITRAN	High-Resolution Transmission molecular absorption database
IR	Infrared
KNMI	Koninklijk Nederlands Meteorologisch Instituut
METOP	Meteorological Operational Satellite
NETCDF	Network Common Data Form, NetCDF
NIR	Near-Infrared
NRT	Near-Real-Time
RAA	Relative Azimuth Angle
RTM	Radiative Transfer Model
SRF	Spectral Response Function
SZA	Solar Zenith Angle
SAA	Solar Azimuth Angle
TOA	Top-of-Atmosphere
UTC	Coordinated Universal Time
UV	Ultraviolet
VIS	Visible
VZA	Viewing Zenith Angle
VAA	Viewing Azimuth Angle

Chapter 8

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Chapter 9

Addendum

9.1 Calculating an AAI equivalent from model data

9.1.1 Assumptions

In the AAI calculation there is a step where the (surface / scene) albedo at 380nm is adjusted to the radiance of the measurement. This step requires knowledge of the measurement (or simulation) before the AAI is calculated. We don't expect that this external information is available to the forward model that feeds the radiances to the IFS.

We are using the following assumptions:

- There is no prior interaction or prior knowledge of the measurement by the regular forward modeling process calculating the radiances.
- The forward model only uses IFS model parameters (and external LUTs).
- There is no iterative process to reach radiative closure at TOA in the IFS
- Changes in atmosphere / surface parameters go via the model via weighting functions and/or adjoint.

9.1.2 RTTOV

Model inputs to RTTOV:

- Surface albedo at 380nm (initial can be GOME-2 or Tropomi or other internal LER)
- Aerosol profile i.e.: distribution as a function of height / pressure of a known type of aerosol

- Spectral properties of aerosol type (phase function, single scattering albedo, or equivalent)
- Ozone profile (because 380 is still a bit sensitive to O3)
- Cloud information (at least: cover and altitude, because it changes the effective albedo compared to the surface albedo). To be tested whether an Independent Pixel Approximation would work for clouded scenes.

Process:

- RTTOV calculates radiances / reflectances at 340 and 380nm, about 1nm wide or at single wavelength
- RTTOV calculates weighting functions / adjoint of aerosol and surface albedo
- Offer those values to IFS and let it do it's magic
- IFS should modify aerosol profile (distribution/density), and the local (clear sky) surface albedo at 380nm (with a slow change permitted (snow/ice?))

Note that the surface albedo at 380nm should be a parameter that IFS tracks internally. The ozone content is already tracked.

9.1.3 Calculating the AAI equivalent

With the calculated values by RTTOV from the previous section, one can follow the normal process of calculating / retrieving an UV AAI value, as if it was the true measurement. See *Tuinder et al.* [2021], for details. This calculation can be an independent verification of how well the forward model represented the observed state of the atmosphere.

9.2 Possible follow up steps

Potential next steps for future follow up projects:

- Check the derivatives from both the RTTOV and DISAMAR models
- Using RTTOV, try out to calculate the AAI using the aerosol with information coming from the IFS and compare this with a real (GOME-2) measurement.
- When the forward modelling workflow is set up, start the monitoring the AAI derived from the IFS/RTTOV with GOME-2 or similar instruments.