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Implementation of UV radiance observation operator in the MOCAGE suite

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Implementation of UV radiance observation operator in the MOCAGE suite

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Introduction

This deliverable deals with the implementation of the Radiative Transfer Model (RTM) DOME (DLR) in the Chemical Transport Model (CTM) MOCAGE (Météo-France/CERFACS) for assimilation of UV radiances. The report covers the implementation and tests of the forward RTM computations and a comparison with GOME-2 Level 1B measurements (misfit analysis). This task represents the first step towards the assimilation of L1 radiances, which will be covered in the follow-up WP3 reports.
The document is structured as follows: Section 1 describes the CTM configuration used for this study and presents a validation of the simulated ozone fields during the period of interest; Level 1 satellite data are presented in Sec. 2; the technical implementation of DOME and its configuration is described in Section 3; Section 4 presents a comparison between simulated and observed reflectance in the GOME-2 ozone window (265-330 nm); the sensitivity of the simulated spectrum to some RTM modeling choices are discussed in section 5. Finally, some conclusions and recommendations are given in Section 6.

1. Chemical transport model

1.1 Model configuration and reference simulations

The CTM used in this study is MOCAGE in its standalone version, as opposed to the integrated IFS(MOCAGE) version. The main objective of WP3 is to demonstrate the feasibility of assimilating UV radiances to improve modeled ozone and compare the performances of this novel approach to the assimilation of Level 2 products. Accordingly with this objective, we considered using a simplified chemistry scheme and a global model configuration that has been already used in a number of published studies (Massart et al. 2012, Emili et al. 2014, Peiro et al. 2018). The chemical scheme is based on a linearized ozone parameterization (Cariolle and Teyssedre, 2007), which provides reasonable ozone fields in the stratosphere and in the UTLS with a very limited computational cost. This configuration is well suited to evaluate the impact of assimilating moderately dense satellite observations thanks to the relatively long lifetime of O_3 (Emili et al., 2014). The main drawback of the linearized scheme is the occurrence of larger ozone biases in the planetary boundary layer, depending on the region or the season (Peiro et al., 2018). Since the sensitivity of GOME-2 UV spectrum to the lowermost tropospheric ozone is also weak, this does not represent a particular issue with regards to the objectives of WP3.
The model horizontal resolution is set to 2 degrees and the vertical grid is composed of 60 hybrid sigma-pressure levels with a model top at 0.1 hPa (approx. 60 km). The model vertical grid matches with the configuration of IFS for ERA-Interim reanalyses, which provide the meteorological forcing for our simulations.
Since this report is focused on misfit analysis, radiative transfer computations have been performed ‘offline’ using the output (in netcdf format) from previous MOCAGE simulations that are already available at CERFACS and well validated. Two CTM simulations discussed by Peiro et al. [2018] have been used as background: i) the first, named **Control**, is a free MOCAGE simulation ii) the second, named **MLS-a**, is a 4D-Var reanalysis where stratospheric profiles from MLS have been assimilated.

The two simulations cover the full period 2008-2014, but for this and all future WP3 reports only the month of September 2010 will be considered. Averaged **MLS-a** model fields for this month are displayed in Figure 1 as well as the total ozone column retrieved by OMI during the same period. We have chosen 2010 because of the strong ENSO event affecting tropospheric ozone distributions, the month of September corresponding to La Nina most extreme phase (Peiro et al., 2018). September represents also an interesting period with regards to the fast dynamics of the Antarctic ozone hole formation.
One of the main differences between assimilating Level 2 products and L1 radiances consists in using a climatological (L2 assimilation) versus a dynamical a-priori (L1 assimilation) in the inversion of the radiative transfer equation. September 2010 should in principle correspond to large deviations of the ozone field from the climatological values, and, therefore, provide an interesting benchmark period for WP3.

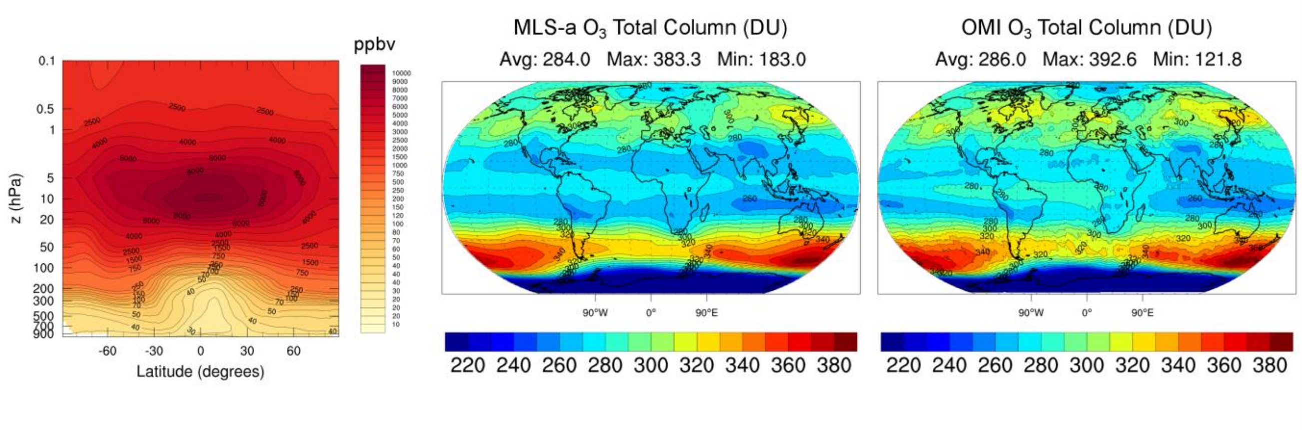

Figure 1: Average ozone fields from the MLS-a analysis for September 2010. Zonal average on the left, total ozone column in the middle. Corresponding average O_3 column retrieved by OMI on the right (OMI-TOMS L3 daily product downloaded from NASA GES DISC archive).

1.2 Validation of reference simulations

Modeled ozone profiles have been validated against all the ozonesondes measurements available during September 2010. The bias and standard deviation for the two reference MOCAGE simulations are displayed in Figure 2 and 3. We remark that the MLS-a shows small biases in the stratosphere (< 5%) and a reduced standard deviation with respect to the control run. The error reduction is very significant at high latitudes in the Southern Hemisphere, where the largest errors occur due to the known limitations of the linearized chemistry scheme with respect to the ozone hole formation mechanism. Tropospheric ozone is in general negatively biased (about 25%), with larger biases occurring at tropical latitudes due to missing emissions and tropospheric ozone chemistry. This preliminary validation characterizes the average performances of the employed CTM and will serve as reference for all future assimilation experiments.
We remind that this report is focused on the comparison of the RTM forward simulations against GOME-2 L1B reflectance. The MLS-a simulation provides here the best option to minimize the impact of ozone profile errors on such comparison, and will let us focus on the analysis of the RTM

configuration and performances. Hence, only the MLS-a simulation will be used further in this report.

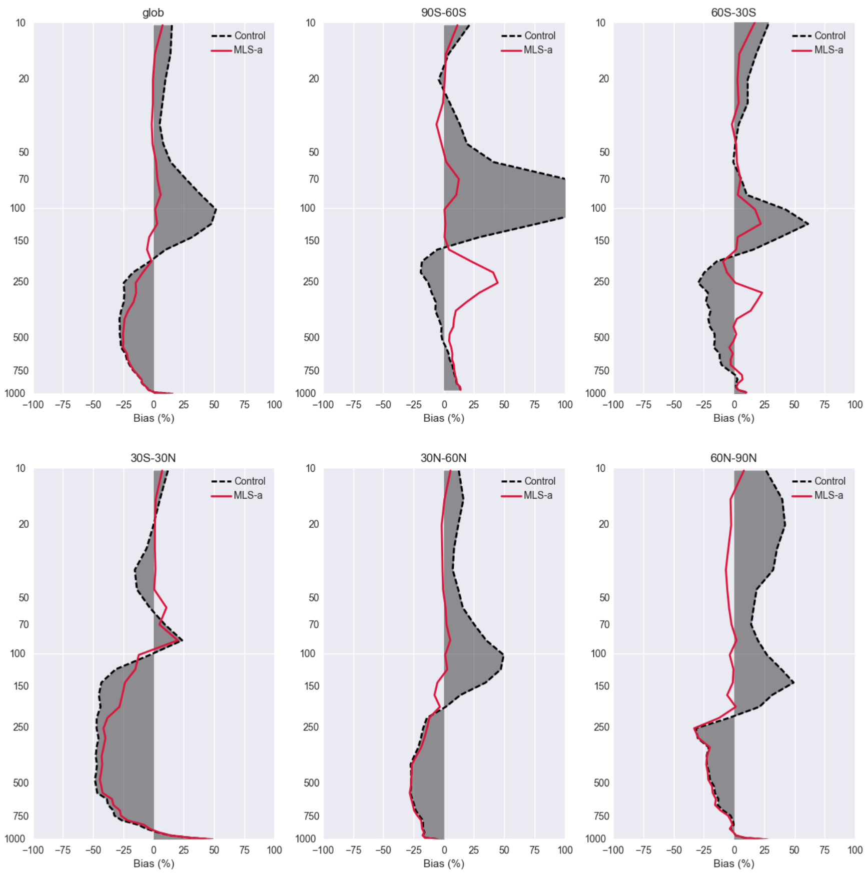

Figure 2: Relative bias (modeled minus measured values) of the MOCAGE control simulation (black dashed line) and MLS-a analysis (red line) against ozonesondes (as percentage of ozonesondes average profiles) for the month of September 2010. First plot on top for the global average and second to sixth plot for five latitude bands separately.

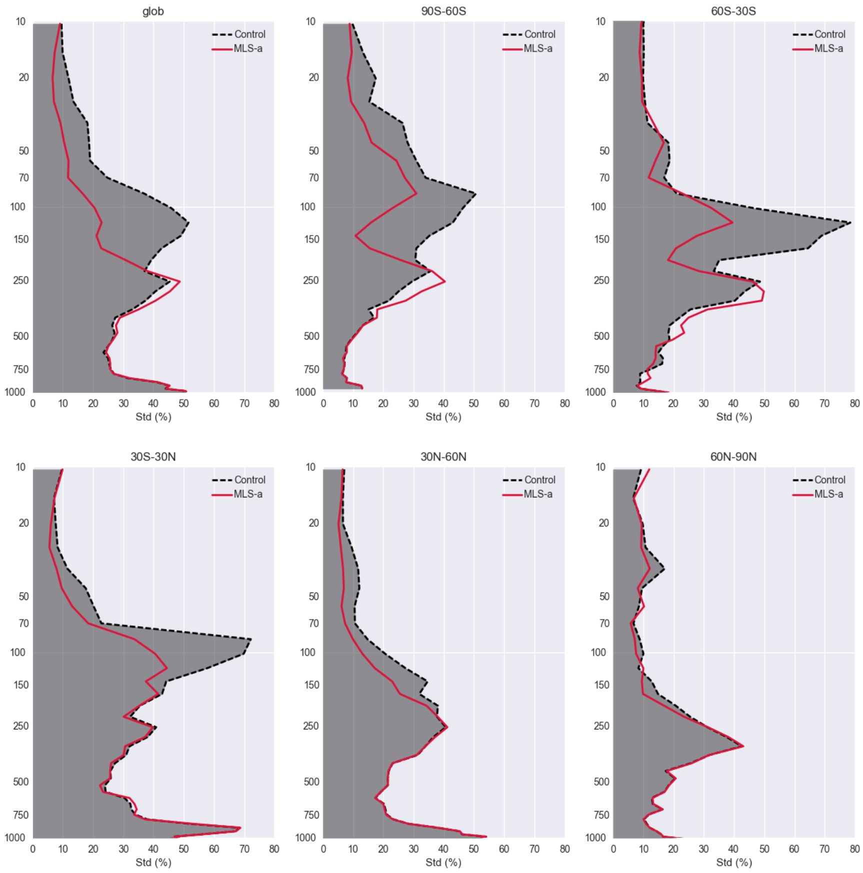

Figure 3: Same as Figure 2 but for the relative standard deviation.

2. GOME-2 Level 1 data

GOME-2 instruments measure Earth's reflected radiation within four main bands covering the Ultra-Violet (UV) and Visible (VIS) spectral regions. The nadir ground-pixel resolution varies from 640x40 km^2 to 40x40 km^2 depending on the spectral band, the satellite platform (MetOP-A/B/C) and the operations period. The nominal operational mode provides 80x40 km^2 pixels for all spectral bands except band 1A, whose pixels are 8 times wider (640x40 km^2). Since July 2013, GOME-2 onboard MetOp-A reduced its swath and increased the nominal ground-pixel resolution to 40x40 km^2 (320x40 km^2 for band 1A). Please refer the official GOME-2 documentation for a detailed description of the bands, spectral and spatial resolutions for the different MetOP platforms. In WP3, we restrict our interest to the Huggins and Hartley ozone bands, which are currently used for operational Level 2 ozone profile retrieval at KNMI (OPERA product) and Rutherford Appleton

Laboratory (RAL product). For L2 ozone profile product description please refer to Keppens et al. [2015] and references therein.

GOME-2 Level 1B data contains geolocalized and calibrated Earth's and sun's spectra for each of the four GOME-2 bands. The needed spectral window (265-330 nm) is located on three distinct bands (1A, 1B and 2B), with the 1A band providing radiances measurements at lower spatial resolution due to longer instrument's integration time.
Official GOME-2 L1B data granules are publicly available at the EUMETSAT Earth Observation Data Portal in native format (GOME-2 GDS Level 1B product). Data granules were downloaded and extracted thanks to the CODA library and the python CODA wrapper made available by DLR to CERFACS. The DLR wrapper allows the extraction of GOME-2 bands raw data. Further pre-processing has been developed at CERFACS to filter missing measurements, compute sun normalized reflectance from radiance values and aggregate the different bands in a single and continuous spectrum for each ground pixel. These preprocessing steps are needed because DOME output is the reflectance measured at the satellite position. The spectral aggregation from multiple bands with different ground-pixel resolutions is needed for Level 2 processing (Van Peet et al., 2014) and will also be adopted here to ease our future comparison with Level 2 assimilation.
A second source of Level 1 data that includes further corrections to the GOME-2 spectra to better account for the instrument degradation, has been provided by KNMI (O. Tuinder). These new data, that we will name hereafter KNMI-L1, should be more accurate than EUMETSAT standard product especially for shorter UV wavelengths. Moreover, KNMI-L1 is used in current OPERA retrievals. When the two approaches will be compared (Level 1 versus Level 2 assimilation) in the second phase of the project, the OPERA L2 retrievals will be used. Using exactly the same L1 spectrum (and its error covariance) within the two approaches is a necessary step to allow a fair comparison of the results.
Differently from EUMETSAT L1B, the KNMI-L1 granules already contain aggregated and normalized spectral reflectance and can be used without need of further pre-processing, except for possible cloud filtering or other data selection criteria.
We plan to use only clear-sky pixels in WP3, to avoid more complex and uncertain RTM computations for this exercise. L1 pixels are therefore filtered based on the "CloudFraction" field available in KNMI-L1 granules, which was computed using the Version 8 of the FRESCO algorithm (Wang et al., 2008). All pixels with a cloud fraction value exceeding 5% are screened and the remaining are named "clear-sky" hereafter. Pixels whose CloudFraction value is missing (e.g. over snow/ice surfaces) are screened as well.
For the period of analysis (September 2010) only the MetOP-A satellite is available. An example of "clear-sky" GOME-2 observations found in KNMI-L1 granules for the 15th September 2010 is displayed in Figure 4. All L1 data are converted to the data format needed for the MOCAGE assimilation system (HDF format).

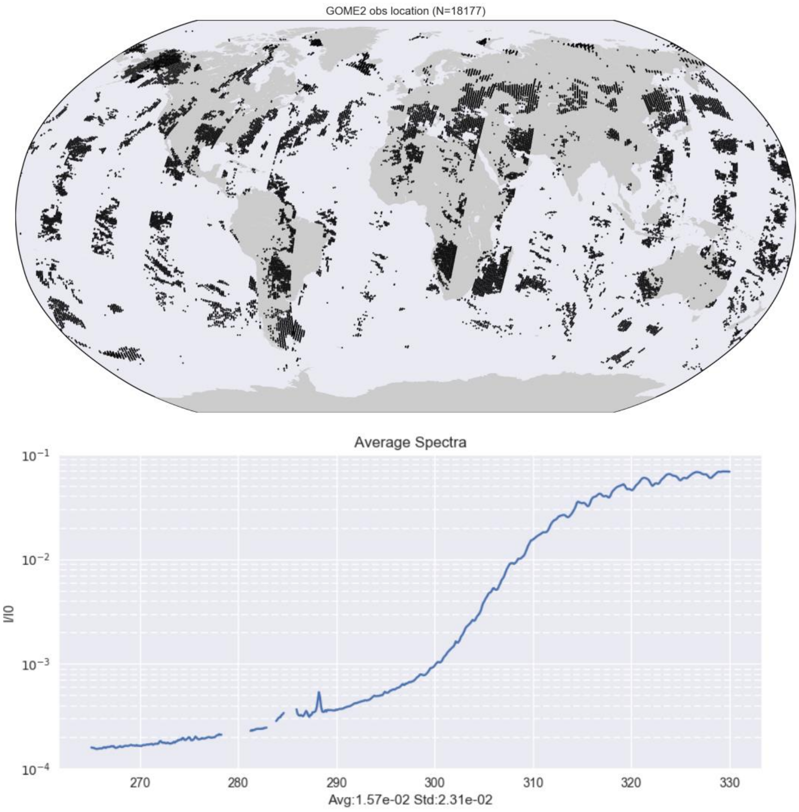

Figure 4: GOME-2 clear-sky measurement locations on 15th September 2010 (top) from KNMI-L1 granules and corresponding average reflectance in the ozone spectral window (bottom).

3. Implementation of DOME RTM in MOCAGE

DOME is a radiative transfer model based on the Discrete Ordinates (DO) method developed at DLR (D. Efremenko) to simulate UV-VIS-IR radiances and perform retrievals of atmospheric profiles and surface properties. Details on the RTM are already given in a separate CAMS42 report (deliverable D42.3.1.1). We discuss here some technical aspects related to the implementation of DOME in the MOCAGE assimilation system.

DOME was delivered to CERFACS as a collection of Fortran 77 routines and its current version is identified with an 'alpha'. The standalone DOME executable that results from compiling the Main.f source code computes the reflectance measured by the satellite for a **single** atmospheric column defined by the user through input ASCII files and/or extraction from climatological database files. In particular, the main user input file defines the ozone profile in volume mixing ratio (vmr) units and the correspondent pressure levels.

The RTM configuration is done through modifications of the Main.f source code, therefore implying the recompilation of the code. One or, optionally, multiple viewing geometries can be computed within a single execution of the code, as well as multiple spectral windows for a given satellite. The RTM computations are well distinguished in a *setup* phase and a numerical integration phase. The *setup* depends, among others, on the height and albedo of the ground pixel, the atmospheric column (pressure, temperature, trace gases) and satellite/sun zenith and azimuth angles. The output, which can optionally include the Jacobian matrix with respect to input profiles and surface properties, is stored in ASCII files.

The DOME code in its initial release form appears well adapted for a processing chain that performs independent RT computations for each ground pixel, with independent input/output files and possibly parallel executions of the main code through operating system directives. However, this is not the case of variational assimilation systems, where all observations contribute simultaneously to the minimization of a global cost function and multiple calls of the RTM computations are needed, for example after computing the analysis or when advancing the simulation in time. In this context, the input/output of the RTM need to be stored on fast random-access memory to avoid the burden of a high number of disk accesses and multiple calls of the RTM with different inputs must be possible within a single execution.

A significant amount of work at CERFACS concerned the adaptation of DOME to overcome these limitations and allow multiple online calls within the MOCAGE data assimilation system. In particular this work concerned the definition of the interfaces to exchange data online with the existent data assimilation code, the introduction of a loop on the RTM input atmospheric profiles - ground pixels and the reorganization of DOME setup and integration calls to avoid redundant operations (e.g. accessing climatological databases for each ground pixel). To facilitate this work, the Main.f was first converted to F90 format and the DOME internal routines grouped and compiled as an external library. Second, the Main.F90 code was reassembled in a new F2003 (Fortran 2003) class of the MOCAGE observation operators (see Table 1 for further details on the implemented procedures). The resulting code allows the correct execution of all operations needed within variational data assimilation:

1) A setup phase that depends only on the RTM static configuration (e.g. choice of simulated wavelengths, modeled and climatological gases), corresponding to the *setup* procedure in Tab. 1;
2) A setup phase that depends either on time (e.g. data extraction from a seasonal climatology), ground pixel location (e.g. surface height) or both (e.g. temperature profile, surface albedo), but not on variables that can be corrected by the assimilation (*build_H* procedure in Tab. 1);
3) A final setup phase that concerns only those variable that the assimilation can correct (e.g. the ozone field), followed by a forward RTM integration (*apply_H* procedure in Tab. 1).

Step 1 is performed only once and should be valid for all assimilation windows and observations. This static configuration is assigned through a new section of the *.json* namelist of the MOCAGE assimilation system. The parameters that can be set through the namelist include:

- the simulated wavelengths;
- the RTM vertical grid;
- the RTM input gases (O_3, NO_2);
- whether to extract the surface albedo and the auxiliary gases from a climatological database, from MOCAGE dynamical fields or from observations input files;
- switches for diagnostic output.

Other RTM options that are still hard-coded in DOME sources and/or not yet activated (e.g. aerosols, clouds, RTM solver options etc.) could be easily added in future whenever needed.

Step 2 is normally performed once at the beginning of each assimilation window, when the number and location of satellite observations become available. Step 3 can be performed multiple times for each assimilation window (e.g. before and after the variational analysis).
Another important modification that has been done to the original version of DOME is the treatment of the input gases in step 3: originally, the user ozone profile given in vmr units on vertical pressure levels was interpolated by DOME internal routines on the vertical RTM grid, which is in meters. However, the Jacobian matrix of the RTM was computed by DOME with respect to ozone partial columns on the RTM grid instead of the original input levels. To perform data assimilation, the linearized observation operator must take as input exactly the same physical quantity of the corresponding non-linear operator. Therefore, the needed vertical interpolation between the MOCAGE and the RTM vertical grids is now performed using dedicated MOCAGE interpolators, and ozone partial columns are computed prior to the RTM call (*vert_interpol* routines in Table 1).
Finally, an efficient hybrid parallelization was implemented to reduce the runtime of RTM computations for application to GOME-2 global observations scenes (about tens of thousands ground pixels per day, see Section 2). The loop on simulated wavelengths inside the DOME forward model routines was parallelized using OpenMP directives, whereas the loop on ground pixels was parallelized using MPI directives. This choice allows an efficient distribution of the RTM computations on standard clusters composed of many-cores nodes, such as those available at CERFACS, Météo-France and ECMWF.

Table 1: Type-bounded procedures of the DOME Fortran 2003 class implemented in MOCAGE

procedure, public :: setup	Static setup of the RTM, includes vertical grid configuration, gases and wavelengths selection
procedure, public :: alloc_obs_data	Allocation of all arrays that depend on the number of observations
procedure, public :: prep_output	Preparation of assimilation output HDF file (groups and datasets)
procedure, public :: Boolmask	Internal procedure for accessing data masks
procedure, public :: read_obs_data	Observations reader from input HDF file
procedure, public :: write_obs_data	Writes assimilation diagnostics on output HDF file
procedure, public :: dealloc_obs_data	Deallocation of all arrays that depend on the number of observations
procedure, public :: build_H	Construction of the space-time interpolators, interpolation of auxiliary data (e.g. temperature) extraction of climatological data (e.g. albedo)
procedure, public :: build_invR	Construction of the observations error covariance matrix $\mathbf{R}^{-1}$
procedure, public :: apply_H	Interpolation of observed fields (e.g. ozone) and call of the RTM solver
procedure, public :: filter_obs	Dynamical observations filter based on misfit values
procedure, public :: apply_H_tl	Interpolation of observed fields and application of the linearized RTM
procedure, public :: apply_H_adj	Adjoint code of apply_H_tl

procedure, public :: apply_invR	Computation of $\mathbf{R}^{-1}\,\mathbf{dy}$ where **dy** is the innovation vector
procedure, public :: Add_Jo	Computation of the J_o term of the variational cost function
procedure, public :: build_vert_interpol	Internal procedure for the construction of vertical interpolators between CTM and RTM grids
procedure, public :: apply_vert_interpol	Internal procedure for the computation of vertical interpolations (equal to linearized code)
procedure, public :: apply_vert_interpol_adj	Adjoint code of apply_vert_interpol
procedure, public :: tl_adj_test	Perform Tangent Linear and Adjoint code tests
procedure, public :: SqrtB_Mult	Compute the $\mathbf{B}^{1/2}\,\mathbf{dx}_o$ where $\mathbf{dx}_o$ is the increment of the augmented control (e.g. for albedo control)
procedure, public :: SqrtB_Mult_Adj	Adjoint code for SqrtB_Mult

Some of this adaptation work was not strictly necessary for the purposes of this report, since only 'offline' RT simulations are presented here. However, this type of implementation is required for the second phase of the project, which concerns online assimilation of L1 data. Hence, we could benefit from the new fully coupled and parallelized MOCAGE-DOME system to run forward RTM computations for the current report and we will rely on these developments and their validation in the follow-up phase of the project.

4. Comparison between simulated and GOME-2 reflectance

This section discusses the results obtained performing forward DOME computations on ozone fields from the MLS-a reanalysis. MLS-a fields are stored every 6 hours. Hence, the MOCAGE observation operator performs both temporal and spatial interpolation to match the satellite observations prior to the application of the vertical interpolator and the RTM operator (see Sec. 3). All presented results are for the 15th September 2010.

4.1 Reference simulation

The reference configuration of DOME used for the presented simulations is summarized in Table 2. The total cost to simulate the 18177 GOME-2 observations shown in Figure 4 is equal to 16.7 hours CPU on Intel Haswell processors (E5-2680v3) at 2.5 Ghz. The cost includes all the O_3 field interpolations, which represent, however, a very marginal percentage of the RTM cost. Such CPU cost exceeds by far the cost of 24 hours-long simulations with typical global configurations of MOCAGE. For example, the cost of the MOCAGE integration for 24 hours with the used configuration (linearized chemistry) is about 0.1 hours CPU. However, distributing the RTM computations on 4 HPC nodes with two sockets on each node composed of 12 cores (96 cores in total), and exploiting both MPI and OpenMP parallelization, reduced the runtime to approximately 11 minutes. Thanks to the property of being "embarrassingly parallel", RTM computations do not represent a runtime bottleneck, as long as enough CPU cores are available. On the other hand, different possibilities exist to reduce the CPU cost of the RTM, e.g. reduce the vertical or spectral resolution, lower the number of discrete ordinates or use information compression techniques within the RTM (PCA). The reference configuration was designed to provide precise results without particular attention to the cost of the simulation. Some of these possibilities will be examined in Section 5.

Table 2

DOME reference configuration	
Vertical grid	21 vertical levels from the surface up to 60 km. Vertical resolution of 2.5 km below 45 km, 5 km above 45 km
Input meteorology	Pressure and temperature from MOCAGE (ERA-Interim)
Input gases	O_3 (MOCAGE), NO_2 (US climatological profile)
Cross-sections	GOME-2 convolved cross section from IUP / University of Bremen (V5.0 for O_3, V2.1 for NO_2)
Spectral range	265-330 nm
Surface Albedo	GOME-TOMS Lambertian-Equivalent Reflectivity (LER) at 335 nm (1° resol., monthly climatology)
Number of Discrete Ordinates	8
Clouds, aerosols, BRDF, polarization, ring effect	Not accounted

Simulated and GOME-2 spectral reflectance are displayed in Figure 5 for different latitude bands. We remark a relatively good correspondence for wavelengths larger than 290 nm. Some spikes are found in GOME-2 spectra between 285 and 290 nm and a systematic bias between the simulation and the measurements appears for shortest wavelengths (< 280 nm).

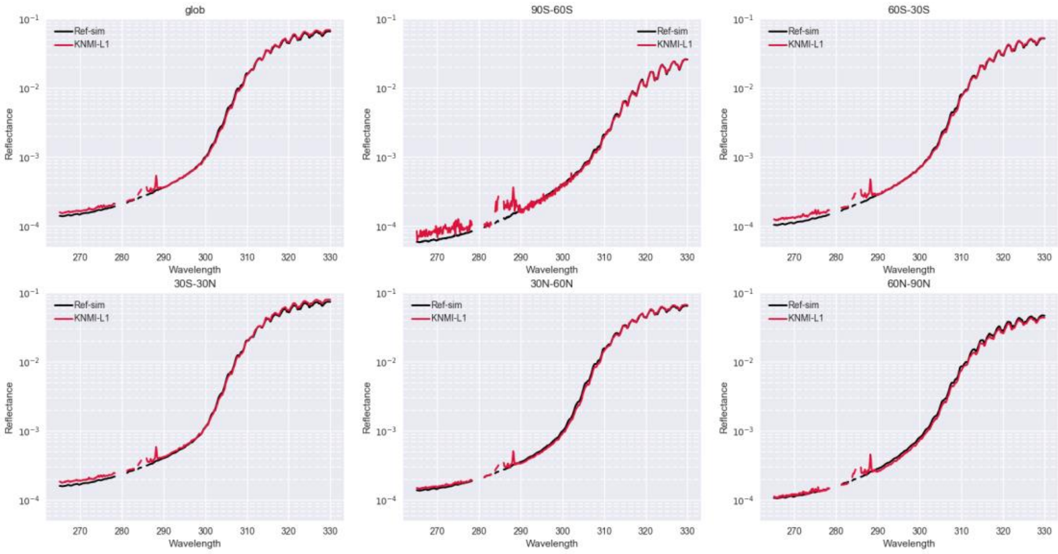

Figure 5: Simulated (black) and GOME-2 (red) spectral reflectance averaged globally (top left plot) and for 5 latitude bands.

Relative bias and standard deviations are displayed in Figure 6 and 7 to highlight the differences found in Figure 5. For $\lambda > 305$ nm we remark that both bias and standard deviation remain generally below 10%. The standard deviation increases significantly for shorter wavelengths, with maximum values of about 60% at approximately 286-288 nm. The bias becomes positive in the 300-310 nm region and reaches the largest (negative) values also at 286-288 nm. Higher standard deviations are expected for short wavelengths due to GOME-2 enhanced instrumental noise. However, the reasons for the larger errors at 286-288 nm and the negative bias for $\lambda < 290$ nm are currently under investigation with the L1 data providers and RTM experts. In particular, the negative bias for $\lambda < 290$ nm appears linked to the top of the modeled atmosphere fixed at 60 km. This aspect is further discussed in Section 5 of this report.

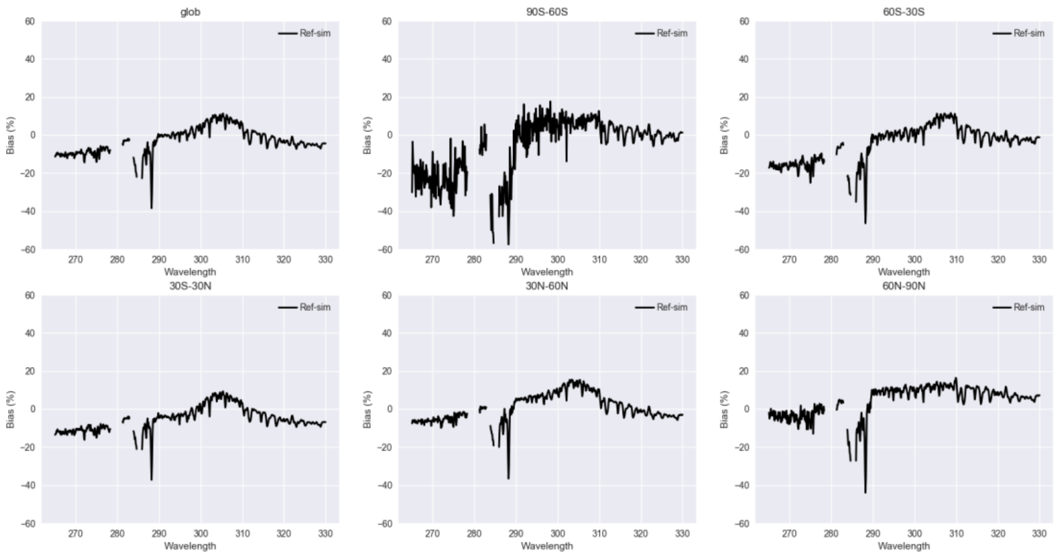

Figure 6: Relative bias between simulated and GOME-2 spectral reflectance shown in Fig. 5, as percentage of GOME-2 reflectance.

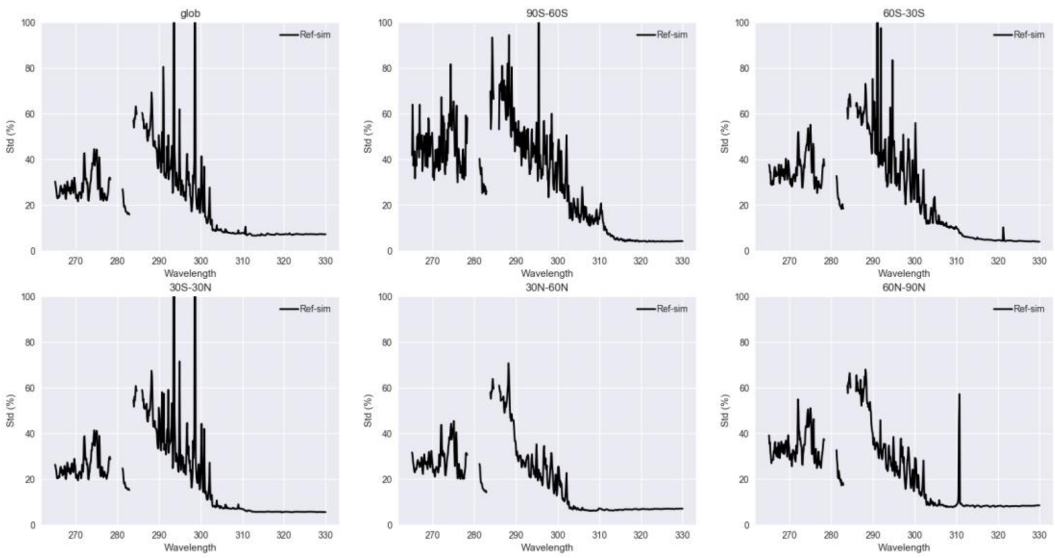

Figure 7: Relative standard deviation between simulated and GOME-2 spectral reflectance shown in Fig. 5, as percentage of GOME-2 reflectance.

Relative differences for individual pixels and a selection of wavelengths are displayed in Figure 8, showing that for shorter wavelengths (< 300 nm) the impact of measurement noise might be very significant for single observations, with relative differences between modeled and GOME-2 reflectance exceeding 100% of the GOME-2 values. These pixels will demand particular care within the data assimilation procedure to avoid possible local degradation of the modeled O_3 field.

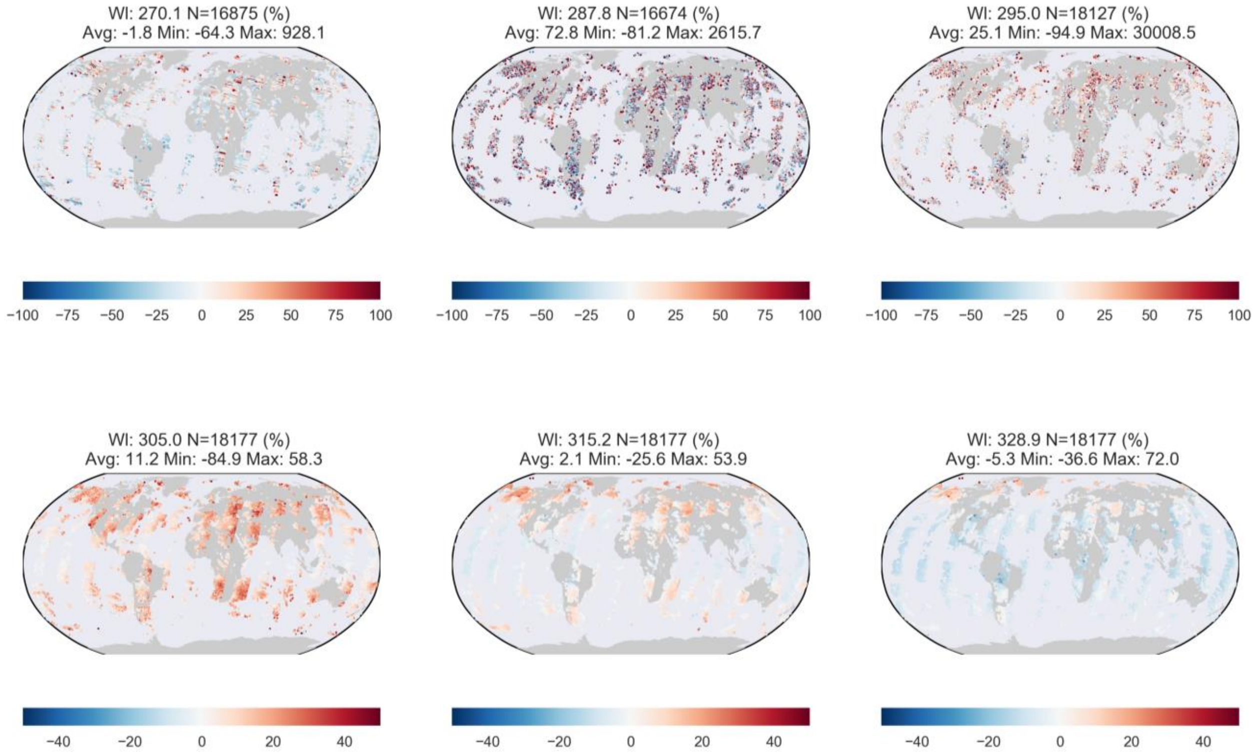

Figure 8: Relative differences between simulated and GOME-2 reflectance (as percentage of GOME-2 values) for all simulated satellite pixels and a selection of wavelengths.

4.2 Eumetsat L1B

The comparison between modeled and measured reflectance has been done also with the Eumetsat L1B product publicly available from the Eumetsat Data Portal. Ground pixels have been first collocated with those available in KNMI-L1 granules, which were masked with respect to missing data and cloudiness. Therefore, exactly the same ground pixels are used for this comparison. The global average biases are shown in Figure 9 and highlight the occurrence of much stronger biases with the Eumetsat L1B. This result confirms the need to preprocess GOME-2 data and account for the instrument degradation prior to data assimilation.

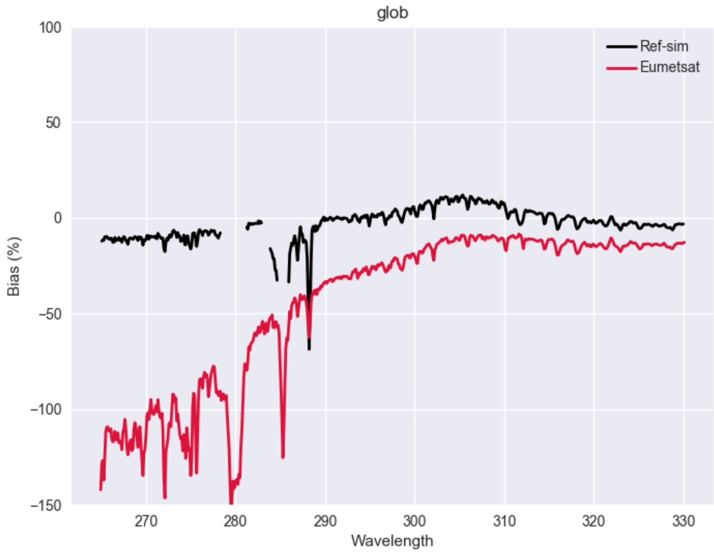

Figure 9: Relative difference between simulated and GOME-2 spectral reflectance as percentage of simulated reflectance for KNMI-L1 data (black) and Eumetsat L1B (red).

4.3 Surface Albedo

An important parameter for UV simulations is the surface albedo, especially at longer wavelengths (> 300 nm). The reference DOME albedo (GOME-TOMS LER) was replaced with the albedo values found in the KNMI-L1 granules (AC-SAF GOME-2 LER product) to check the sensitivity of the results to the albedo values. The new results are compared with the reference in Figure 10. We remark that the original negative bias in the 310-330 nm spectral region is significantly reduced on a global base, the strongest reduction being for mid- and low-latitudes. Hence, the AC-SAF surface albedo will be used in future analyses. This choice will also further reduce discrepancies between assimilation of L1 and L2 in the follow-up phase of the project.

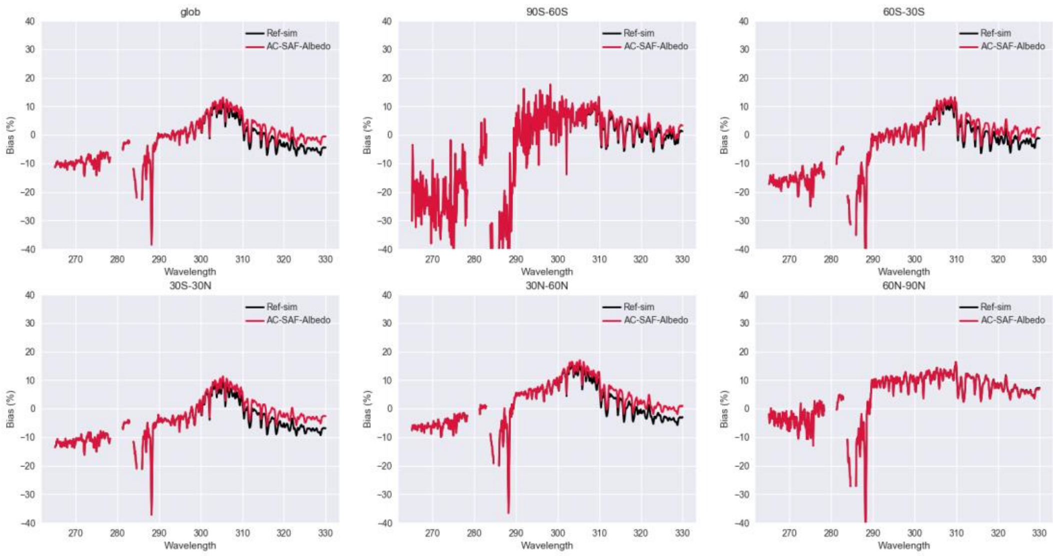

Figure 10: Relative differences between simulated and GOME-2 spectral reflectance as percentage of GOME-2 reflectance for two different surface albedo databases (reference simulation with GOME-TOMS LER in black, AC-SAF GOME-2 LER in red).

5. Sensitivity tests to RTM configuration

5.1 RTM vertical grid

The vertical discretization used for the RTM computations is a critical aspect of the system configuration. A coarser grid decreases the CPU cost of the RTM, whereas a finer grid can improve the precision of the RTM computations and, within DA, permit to better retrieve local features of the O_3 vertical distribution. For example, the OPERA GOME-2 ozone is retrieved on 40 layers from the surface up to 0.001 hPa.

In principle, setting the vertical discretization of the RTM close or equal to the CTM one should represent the best option for radiances assimilation. However, the finite spectral resolution of the instrument, the presence of instrumental noise and the vertical spread of RT Jacobians all limit the capacity to retrieve too detailed vertical profiles, no matter how fine the RTM resolution can be. Therefore, a better option for operational systems might be to lower the vertical resolution of the RTM and search a good compromise between the (already high) RTM cost and the precision of the results. This is particularly important in case of operational CTMs with very large number of vertical levels (> 50). In this section we compare the results obtained changing the RTM vertical grid with respect to the reference simulation (Sec. 4.1).

The following grids have been used:

- A “Coarse” grid with halved vertical resolution compared to the reference simulation (11 levels, 5 km resolution below 45 km, 7.5 km above 45 km);

- A “Fine” grid with doubled vertical resolution (42 levels, 1.25 km resolution below 45 km, 2.5 km above 45 km);
- An “Adaptive” grid that makes the optical thickness of the different O_3 partial columns more homogenous (23 levels, 2.5 km resolution below 15 km, 1.5 km from 15 km to 36 km, 6 km from 36 km to 48 km and 12 km above). This choice should improve the convergence of the RTM solver.

The global average bias for the reference choice and the above grids is displayed in Figure 11. We remark that the impact of the vertical resolution becomes significant for $\lambda < 310$ nm, due to the increased sensitivity of the reflectance to the O_3 profile. The coarser grid decreased the cost of the simulation from 16.7 to 9.2 CPU hours but increased the bias between modeled and measured reflectance to more than 10% in the 300-310 nm range. The fine grid gives the best results in this spectral region, but doubles the simulation cost to 33.6 CPU hours. The “adaptive” grid provides very close results to the reference for $\lambda > 300$ nm but improves the fit for shorter wavelengths ($\lambda < 280$ nm), demanding only slightly more computations (18.4 CPU hours) than the reference.

All previous RT simulations used the same Top Of Atmosphere (TOA) as MOCAGE, which sits at 60 km or approximately 0.1 hPa. We extended the MOCAGE atmosphere above 60 km to verify if we could reduce the negative biases observed for shorter wavelengths (Sec. 4 and Fig. 11). The MOCAGE temperature and pressure profiles have been completed with the US standard atmospheres up to 90 km (approx. 0.001 hPa) depending on season and latitude. The O_3 profile has been extended to 90 km based on MLS global average profile (up to 0.01 hPa, extrapolated above) computed using all observations available on 15th September 2010. The DOME NO_2 climatology, being already available up to 100 km, did not require any special treatment. The results for the 0-90 km RT simulations using both the reference and “Fine” vertical resolutions are displayed in Fig. 12 and compared with previous simulations. We remark that the negative bias is significantly reduced with both the Ref-90km and Fine-90km configurations when compared to the corresponding 0-60 km simulations. Moreover, the Fine-90km configuration gives now better results than the reference one also for $\lambda < 300$ nm, which seems more coherent than the behavior in Fig. 11. Since the added layers above 60 km are modeled using a coarse resolution of 10 km, the total number of RTM levels and the CPU cost increased only marginally (20.5 CPU hours for Ref-90km instead of 16.7 for the reference configuration, 34.9 CPU hours for the Fine-90 km instead of 33.6 for the Fine configuration).

It is difficult to draw final conclusions about the best RTM grid option prior to extensive DA tests because part of the biases in Figure 11 and 12 might be due to other reasons (e.g. tropospheric ozone biases in MLS-a). However, the main conclusion to be retained here is that there is a significant sensitivity of the results to the vertical resolution and extension of the RTM grid. A future report will contain a detailed analysis on the impact of the vertical grid on data assimilation results.

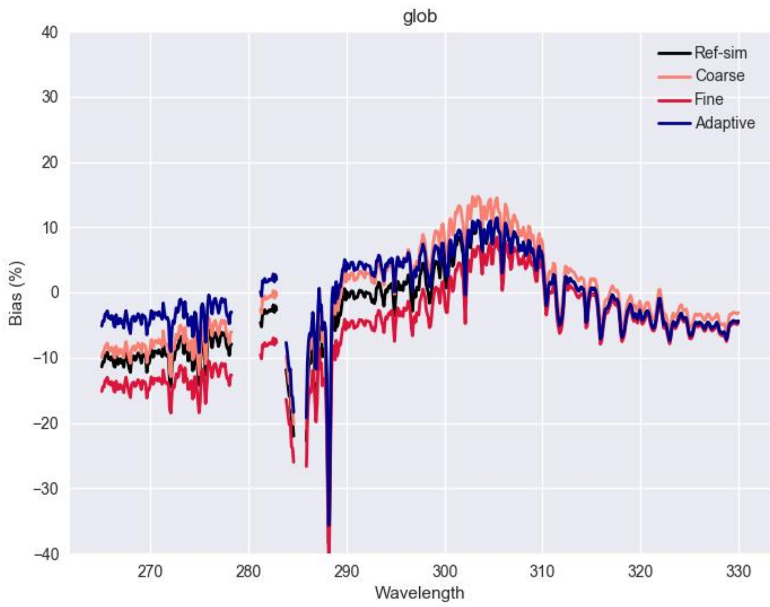

Figure 11: Relative differences between simulated and GOME-2 spectral reflectance as percentage of GOME-2 reflectance for different vertical resolutions of the RTM computations.

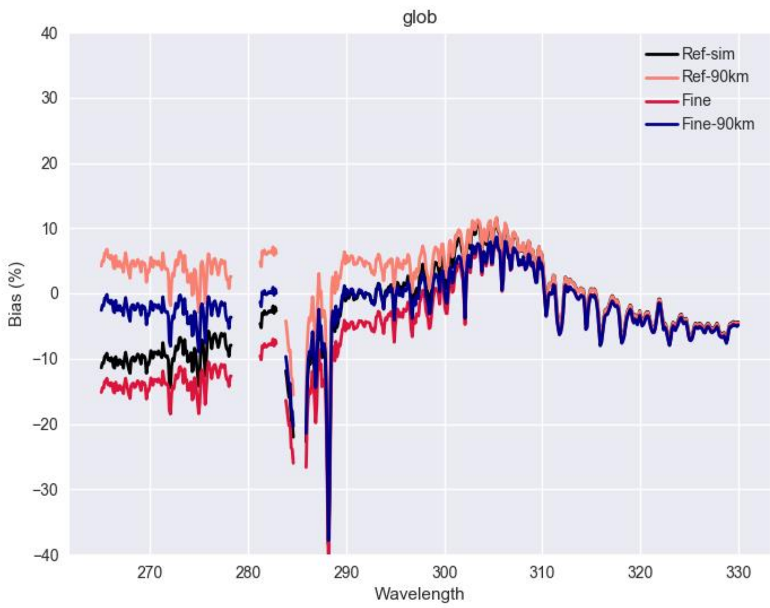

Figure 12: Relative differences between simulated and GOME-2 spectral reflectance as percentage of GOME-2 reflectance for two different vertical resolutions (reference and fine) and top of the atmosphere (60 km and 90 km).

5.2 Number of discrete ordinates

The number of Discrete Ordinates (DO), which represents the angular discretization of the RT problem, is another key parameter of the RTM configuration. Depending on the scattering properties of the traversed medium, the DO number can significantly affect the precision of the RT computations. We made the number of DO vary from 2 to 16 from the original value of 8, using the most precise and expensive RTM configuration found so far (Fine-90km simulation of previous section). We evaluated the dependence of the results and the CPU cost to this parameter. The simulation cost varied from 11.4 CPU hours with only 2 DO to 105.9 CPU hours when using 16 DO. We could not measure a significant impact on the results, except for a slight (1-2%) bias increase in the case of DO equal to 2 and only for λ > 300 nm. We will consider a number of DO equal to 4 for initial DA tests, which will lower the RTM cost to 16.3 CPU hours instead of the 34.9 CPU hours needed previously with the Fine-90km configuration. Such a low number of DO seems sufficient for the 265-330 nm spectral window and when only O_3 and NO_2 are modeled within the RT. A higher number of DO might be needed if aerosols or clouds were included in the RTM.

6. Conclusions

This report summarizes the work done at CERFACS during the first phase of WP3. This task covered: i) the implementation of the DOME forward RTM operator in MOCAGE for the simulation of GOME-2 UV reflectance ii) the evaluation of results against real data. It included the preliminary steps for all upcoming DA experiments, i.e. the second phase of WP3.
The period of September 2010 has been chosen for the particular O_3 features associated to the formation of the ozone hole and a strong La Nina condition. The accuracy of modeled O_3 fields has been discussed for both a free model configuration (control) and a more realistic reanalysis (MLS-a). The same model configuration will be used initially for future DA experiments. Possible evaluation of more complex/costly MOCAGE configurations will be considered, whenever this appears beneficial for the scope of this study.
The largest part of the achieved developments consisted in:

- preprocessing GOME-2 L1 data from two data providers (Eumetsat and KNMI);
- adapting the original DOME code for an efficient integration in a variational DA environment.

The ensemble of these developments will also serve for all future DA experiments. A number of experiments have been performed to validate the new tools, evaluate the differences between simulated and GOME-2 clear-sky reflectance (misfit) in the 265-330 nm spectral region, and estimate the numerical cost of RT modeling.
Using a reference RTM configuration based on 21 vertical levels and 8 discrete ordinates the spectral misfits (bias and standard deviation) are in accordance with the accuracy of the underlying O_3 field and the GOME-2 instrumental noise. The presence of residual spikes in the KNMI-L1 data in the 286-288 nm region demands further investigation. We have found in general much larger biases using Eumetsat L1B data, which confirms the absolute need to correct for the GOME-2 degradation before any usage of L1B data. Similarly, it is suggested not to use the original GOME-TOMS 335 nm surface albedo climatology, since misfit biases are larger than with the AC-SAF GOME-2 albedo. These results favor using the KNMI-L1 data and surface albedo for the future DA experiments.

Moreover, this choice will allow a stricter comparison between the assimilation of L1 reflectance and L2 profiles from the OPERA product (KNMI). Some particular care might be needed to avoid assimilating individual pixels that show a very noisy behavior for shorter wavelengths.
The numerical cost of the RTM is significant, reaching 16.7 CPU hours for the reference global GOME-2 scene simulated for this report, i.e. approximately 3.3 CPU seconds for each simulated spectrum. The numerical cost will even increase when the computation of the RT Jacobians will be activated within DA experiments. However, the RTM computations can be easily parallelized: using a hybrid OpenMP-MPI parallelization the runtime have been reduced to about 11 minutes on 4 HPC nodes (96 CPUs).
We reckon the vertical grid as being a critical aspect of the RTM configuration due to its impact both on CPU time and resulting reflectance. For example, extending the RT computations above the MOCAGE 60 km top has been found important to reduce the biases for shorter wavelengths (< 280 nm) and increasing the vertical resolution to 1.25 km below 45 km reduced the biases for $\lambda < 310$ nm. Therefore, we recommend reanalyzing the impact of the vertical discretization on DA results.
No strong dependence on the number of DO was found, suggesting that it might be possible to lower the number of DO to 4 for O_3 assimilation.

7. References

Cariolle, D., & Teyssedre, H. (2007). A revised linear ozone photochemistry parameterization for use in transport and general circulation models : multi-annual simulations. Atmospheric Chemistry and Physics, 7, 2183–2196.

Emili, E., Barret, B., Massart, S., Le Flochmoen, E., Piacentini, a., El Amraoui, L., … Cariolle, D. (2014). Combined assimilation of IASI and MLS observations to constrain tropospheric and stratospheric ozone in a global chemical transport model. Atmospheric Chemistry and Physics, 14(1), 177–198. https://doi.org/10.5194/acp-14-177-2014

Keppens, A., Lambert, J. C., Granville, J., Miles, G., Siddans, R., Van Peet, J. C. A., … Zehner, C. (2015). Round-robin evaluation of nadir ozone profile retrievals: Methodology and application to MetOp-A GOME-2. Atmospheric Measurement Techniques, 8(5), 2093–2120. https://doi.org/10.5194/amt-8-2093-2015

Massart, S., Piacentini, A., & Pannekoucke, O. (2012). Importance of using ensemble estimated background error covariances for the quality of atmospheric ozone analyses. Quarterly Journal of the Royal Meteorological Society, 138(665), 889–905. https://doi.org/10.1002/qj.971

Peiro, H., Emili, E., Cariolle, D., Barret, B., & Le Flochmoën, E. (2018). Multi-year assimilation of IASI and MLS ozone retrievals: variability of tropospheric ozone over the tropics in response to ENSO. Atmospheric Chemistry and Physics, 18(9), 6939–6958. https://doi.org/10.5194/acp-18-6939-2018

Van Peet, J. C. A., Van Der A, R. J., Tuinder, O. N. E., Wolfram, E., Salvador, J., Levelt, P. F., & Kelder, H. M. (2014). Ozone profilE retrieval algorithm (OPERA) for nadir-looking satellite instruments in the UV-VIS. Atmospheric Measurement Techniques, 7(3), 859–876. https://doi.org/10.5194/amt-7-859-2014

Wang, P., Stammes, P., Van Der A, R., Pinardi, G., & Van Roozendael, M. (2008). FRESCO+: An improved O2A-band cloud retrieval algorithm for tropospheric trace gas retrievals. Atmospheric Chemistry and Physics, 8(21), 6565–6576. https://doi.org/10.5194/acp-8-6565-2008

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