CAMS Service Evolution

D1.1 Report on construction of AVRAS prototype

Due date of deliverable	31 May 2024
Submission date	23 May 2024
File Name	CAMEO_D1.1_v1.0
Work Package /Task	WP1 Task 1.1
Organisation Responsible of Deliverable	ECMWF
Author name(s)	Samuel Quesada-Ruiz, Angela Benedetti
Revision number	1
Status	Issued
Dissemination Level	PUBLIC

Funded by the European Union

The CAMEO project (grant agreement No 101082125) is funded by the European Union.
Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the Commission. Neither the European Union nor the granting authority can be held responsible for them.

1 Executive Summary

This report describes the first 18 months of activity related to the creation of a prototype assimilation system for aerosol-affected visible radiances (AVRAS) within the Integrated Forecast System's 4DVar in atmospheric composition configuration (IFS-COMPO). The work in these first months has focused mainly on the creation of the infrastructure in a configuration as close as possible to the operational one. The objective of this report is to record the progress made so far and to highlight initial results from the monitoring experiments as well as outline the way forward for the completion of Task 1.1.

The initial efforts have been focusing on four main aspects: (i) the creation of a BUFR template for the visible radiance observations and the development of the buf2odb software which is necessary for the operational implementation; (ii) the inclusion of aerosol fields from the IFS-COMPO for the first time in the radiative transfer interfaces which are used operationally for assimilation of radiances in the IFS; (iii) the testing of the accurate radiative transfer solver (Discrete Ordinate Method, DOM) in monitoring experiments for the month of September 2021 using aerosol and cloud-affected radiances; and (iv) preparations for the inclusion of a new version of the fast radiative solver (RTTOV) which will include a fast solver for aerosol-affected visible radiances (MFASIS-Aerosol).

The BUFR template for visible reflectances has been created and it is in the pipeline for approval by WMO. This has involved the definition of new variables, such as reflectance, which had not been previously defined nor used in an assimilation context.

Prognostic aerosol fields produced in a composition run of the IFS have been "connected" to the radiative transfer interfaces used in operational assimilation. This has allowed the testing of the development using the accurate DOM method and observed reflectances form the Ocean Land Colour Instrument which is an instrument on board of Sentinel3-A/B to generate differences between model first guess fields and the observations. This is a first step towards testing the assimilation. The whole month of September was investigated in this monitoring runs revealing interesting structures in both aerosol and cloud-affected reflectances. Assimilation experiments depend on the implementation of MFASIS-Aerosol which is the fast radiative transfer code for aerosol reflectances. This software will be released in June for the forward operator and later in the year for the tangent linear and adjoint operators. While waiting for this release preparations have been made to accommodate the new software by upgrading to the latest release of the RTTOV package (v14).

Once the full MFASIS-Aerosols with assimilation capability will available and integrated in RTTOV v14, the first assimilation experiments will be run. At this stage, we will consider the option to use level 1 reflectances and screen the cloud-affected pixels using a thresholding method or to use level 2 cloud-cleared reflectances provided for example by NASA for the MODIS and VIIRS instruments. Either approach will bring us a step closer to the assimilation of aerosol-affected visible reflectances in a global air pollution model.

Table of Contents

2 Introduction

2.1 Background

Monitoring the composition of the atmosphere is a key objective of the European Union's flagship Space programme Copernicus, with the Copernicus Atmosphere Monitoring Service (CAMS) providing free and continuous data and information on atmospheric composition.

The CAMS Service Evolution (CAMEO) project will enhance the quality and efficiency of the CAMS service and help CAMS to better respond to policy needs such as air pollution and greenhouse gases monitoring, the fulfilment of sustainable development goals, and sustainable and clean energy.

In the context of aerosol assimilation, progress towards assimilating visible radiances has been made within the ARAS (Aerosol Radiance Assimilation Study) project funded by ESA from 2018 to 2020. It was shown (Figure 1) that the assimilation of level 2 aerosol using visible radiances increases the aerosol load in the analysis to a level comparable to the MODIS aerosol optical depth data and improves other aerosol parameters too.

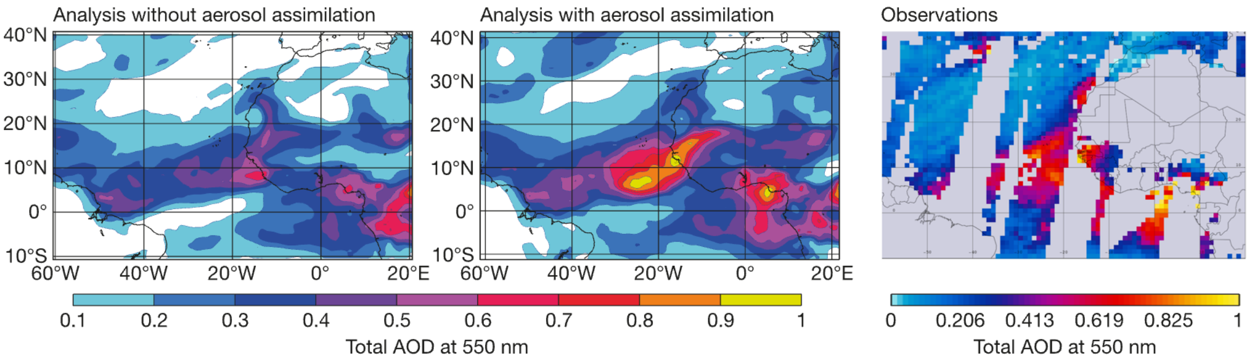


Figure 1. Total AOD at 550 nm analysis without aerosol assimilation (left) and with aerosol assimilation (middle), compared to observed values from MODIS (right).

The infrastructure for visible reflectance aerosol assimilation that will be exploited in CAMEO will rely upon RTTOV-MFASIS AEROSOLS, which is being developed by DWD/LMU using a two-layer model. It is expected to have a beta release for monitoring purposes at the end of Q2 2024 and the final version in Q3 2024. MFASIS-Aerosols will follow a similar scheme that the one used for MFASIS-Clouds (see Figure 2), ie. based on a neural network approach with training data provided by an accurate solver (DISORT). DISORT calculations assume the water cloud is between 2-4 km and the ice cloud is between 6-8 km. MFASIS-Aerosols is being developed in a similar way with a two-layer scheme to address presence of boundary layer aerosols and middle-tropospheric plumes. More details on MFASIS-Aerosols will be provided in the final report.

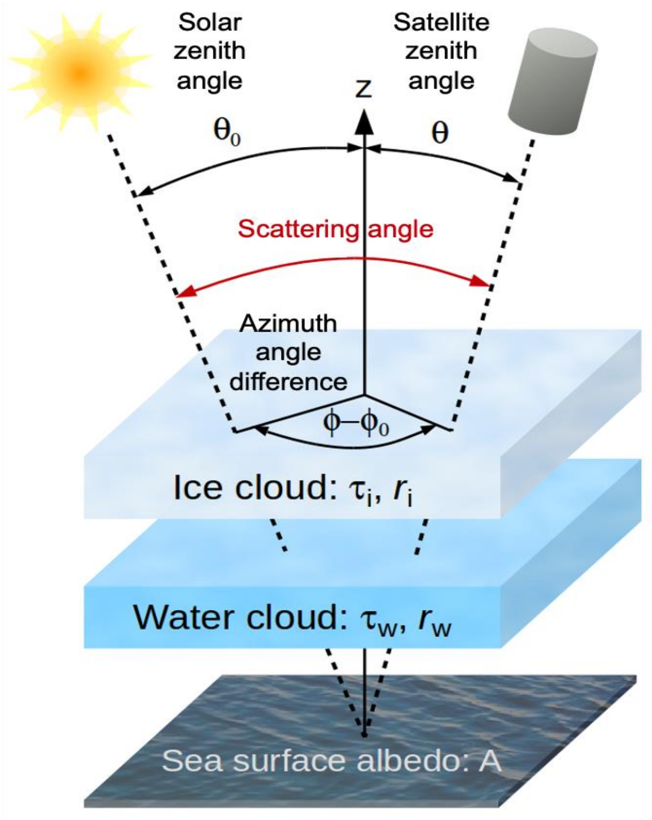


Figure 2. RTTOV-MFASIS Cloud scheme.

Current visible reflectance simulations using RTTOV-MFASIS Cloud show a good performance when compared to observations, but there is a clear lack of aerosol information that we plan to fill within CAMEO. As an example, we can see in Figure 3 that the Saharan dust travelling over the Atlantic is missing in the simulated reflectances.

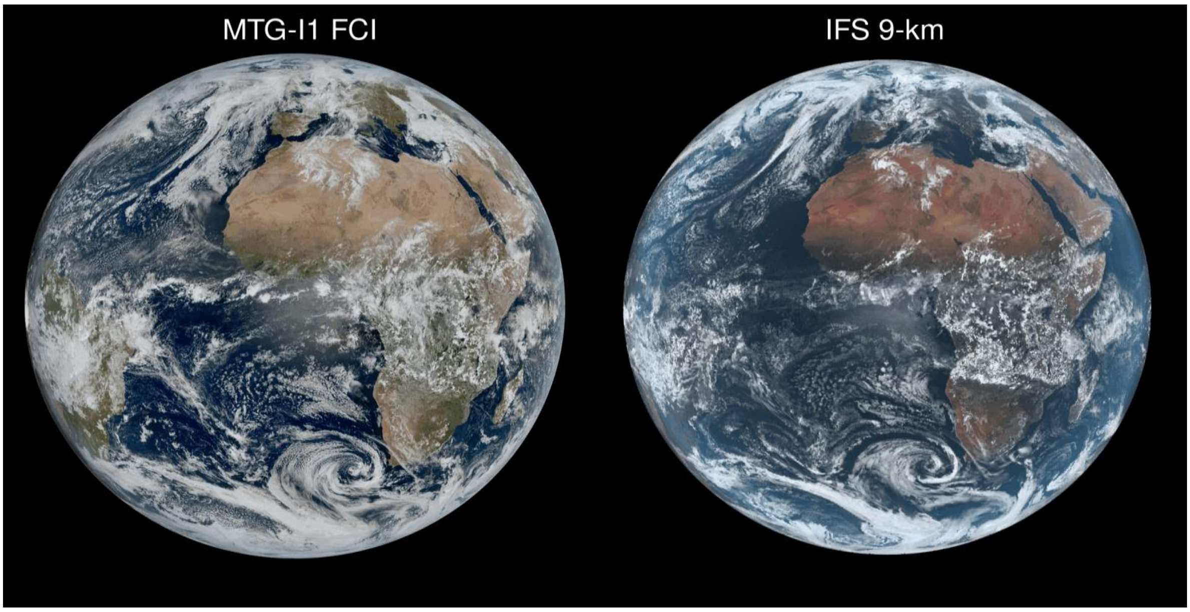


Figure 3. MTG-I1 FCI observations (left) vs IFS-9km reflectances simulated using MFASIS-Cloud (right). Credits: Philippe Lopez (ECMWF).

2.2 Scope of this deliverable

2.2.1 Objectives of this deliverable

This report describes the first 18 months of activity related to the creation of a prototype assimilation system for aerosol-affected visible radiances (AVRAS) within the Integrated Forecast System's 4DVar in atmospheric composition configuration. The work in these first months has focused mainly on the creation of the infrastructure in a configuration as close as possible to the operational one. The objective of this report is to record the progress made so far and to highlight initial results from the monitoring experiments as well as outline the way forward for the completion of Task 1.1.

2.2.3 Work performed in this deliverable

In this deliverable the work as planned in the Description of Action (DoA, WP1 T1.1) was performed. The initial efforts have been focusing on four main aspects:

1. the creation of a BUFR template for the visible radiance observations and the development of the buf2odb software which is necessary for the operational implementation
2. the inclusion of aerosol fields from the IFS-COMPO for the first time in the radiative transfer interfaces which are used operationally for assimilation of radiances in the IFS
3. the testing of the accurate radiative transfer solver (Discrete Ordinate Method, DOM) in monitoring experiments for the month of September 2021 using aerosol and cloud-affected radiances
4. preparations for the inclusion of a new version of the fast radiative solver (RTTOV) which will include a fast solver for aerosol-affected visible radiances (MFASIS-Aerosol).

These four points will be discussed in detail in the next sections.

2.2.4 Deviations and countermeasures

No deviations have been encountered.

3 BUFR template for visible radiances

A full definition of the BUFR form is given in WMO Manual on Codes, Volume I, International Codes, Part B-Binary Codes, WMO-No.306, FM 94-IX Ext. BUFR. In what follows a brief description of the basic structure and representation of the BUFR code is provided.

The BUFR form is a binary representation of meteorological data. It is a continuous bit stream made up of a sequence of octets (one octet is eight bits). The only part of BUFR where information does not end on byte boundaries is the data section, where a length of BUFR table B elements can have any number of bits (although it must not exceed the number of bits in a computer word for non-character data).

The representation of data in the form of a series of bits is independent of any particular machine representation. It is important to stress that the BUFR representation is not suitable for data visualisation without computer interpretation.

The data section consists of one or more data subsets of related meteorological data which are defined, described and represented by a single BUFR table D entry. For observational data, one subset corresponds to one observation. The data section can be in compressed or uncompressed form.

All meteorological data which are assimilated in the ECMWF's 4D-Var have to be converted from their native format into BUFR. This is to ensure operational resilience and reproducibility since the BUFR is fully supported operationally at ECMWF and it is a standard WMO-approved format. Since all operational Numerical Weather Prediction (NWP) centres use observations in this format, it also facilitates exchange of observations between data providers and NWP centres as well as among the centres themselves.

If observations have never been used operationally in an NWP context, very often they do not have a BUFR template associated with them. This is for example the case for visible radiances which have never been monitored or assimilated so far in this context. The CAMEO project aims at making a step forward in the exploitation of these rich datasets by including for the first-time aerosol-affected visible radiances in the IFS-COMPO 4D-Var assimilation which is the basis for the Copernicus Atmosphere Monitoring Service (CAMS) forecasts. To this end, work has been going on in WP1 to create a generalised BUFR template for visible radiances and reflectances. For the moment this template is only internal at ECMWF, but once tested it will be submitted to WMO for official acceptance.

4 RTTOV interfaces with aerosol fields

The aerosol fields from the IFS-COMPO have been included for the first time in the radiative transfer interfaces which are used operationally for assimilation of radiances in the IFS. This allows to account for model aerosols in the radiative transfer calculations to produce the model equivalent of the satellite observed reflectances.

There are currently 9 CAMS aerosol species defined in RTTOV: Hydrophobic Black Carbon (Hydrophobic BCAR), Dust bin 1 (DUS1), Dust bin 2 (DUS2), Dust bin 3 (DUS3), Sulphate (SULP), Sea Salt bin 1 (SSA1), Sea Salt bin 2 (SSA2), Sea Salt bin 3 (SSA3) and Hydrophilic Organic Matter (Hydrophilic OMAT).

It is worth clarifying that at this stage of the project, and in order to progress in parallel as fast as possible, this development has been implemented in the current operational version of the radiative transfer model (RTTOV v13). However, they will need to be adapted to RTTOV v14 as MFASIS-Aerosols, which is being developed by DWD and will be exploited in CAMEO, will only be available in this version.

For the time being we focus on sea surfaces only. MFASIS (and DOM in this case) assumes a Lambertian surface with an albedo given by π times the surface bidirectional reflectance distribution function (BRDF). BRDF values are taken from the input to RTTOV, which in our case is from an RTTOV-internal BRDF model. Over sea surfaces the BRDF due to sun-glint is calculated (Matricardi, 2003) and added to a BRDF derived from USGS water reflectance spectra (Clark et al., 2007). These USGS spectra are returned by the BRDF atlas for sea surface profiles.

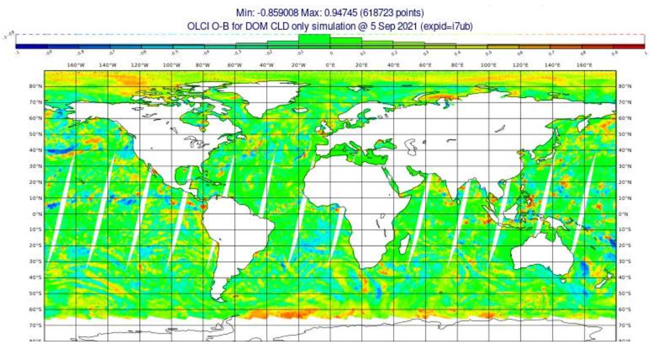
The most relevant code changes required to include aerosols are described here. The main switch to activate the aerosol (and/or cloud) calculation for a given instrument is controlled in arpifs/module/sats_mix.F90. A specific variable number (varno) for 'visible spectral reflectances' was added in arpifs/op_obs/hop.F90 and obsop_rad.F90. In arpifs/op_obs/radtr_ml.F90, the model profiles for these 9 CAMS aerosol species are read and passed to the RTTOV_EC call through the ZPROF variable. In satrad/rttov/ifs/rttov_ec.F90, these values are transformed from level quantities to layer quantities and passed to RTTOV via profiles(j)%aerosols. RTTOV calculation options are set in satrad/rttov/ifs/rttov_ec_setopts.F90. ifsaux/module/rttov_ec_mod.F90 has been extended to include the aerosol mapping between the IFS and RTTOV variables.

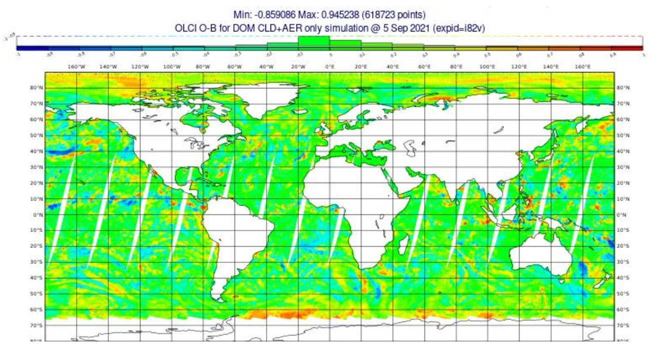
5 Initial tests with an accurate solver

In order to be able to run some tests while the development and testing of the BUFR for visible reflectance is ongoing, it was decided to use Ocean and Land Colour Instrument (OLCI) visible reflectances for the month of September 2021 through the experimental observation framework.

Since MFASIS-Aerosols is not yet available, it was decided to test the implementation for the aerosol calculation using the accurate radiative transfer solver (Discrete Ordinate Method, DOM) available on RTTOV v13 in monitoring experiments for the month of September 2021 using aerosol and cloud-affected radiances from OLCI and the current operational IFS cycle (CY48R1). We used 12 streams for the DOM runs, which is considered to be sufficient to have accurate simulations without the penalty of a higher computational cost.

The OLCI reflectances at 0.64 microns used in this test are not cloud-cleared nor aerosol-cleared, ie. they contain both cloud and aerosol signals. Figure 4 shows the observation minus background (model equivalent) departures for 3 experiments using DOM to simulate: i) only aerosols, ii) cloud and aerosols, and iii) only clouds. It can be seen that cloud is the dominating signal and therefore CLD+AER and CLD are very close (although not identical). Large positive departures in AER are clouds observed by OLCI but not simulated by DOM (since it is an aerosol only simulation). The results for Sentinel 3A and Sentinel 3B are consistent.





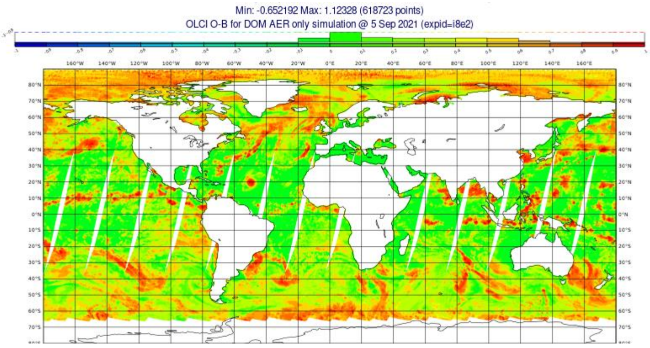


Figure 4. OLCI on Sentinel 3A and 3B O-B departures at 0.64 microns for cloud only (top), cloud and aerosol (middle) and aerosol only (bottom) DOM simulations in CY48R1 on 5 Sep 2021.

A closer look over the Atlantic for OLCI observations and IFS simulated aerosol reflectances is shown in Figure 5. It can clearly be seen the aerosol circulation around and in the vicinity of hurricane Larry (when it was at peak strength) on the 5th September 2021.

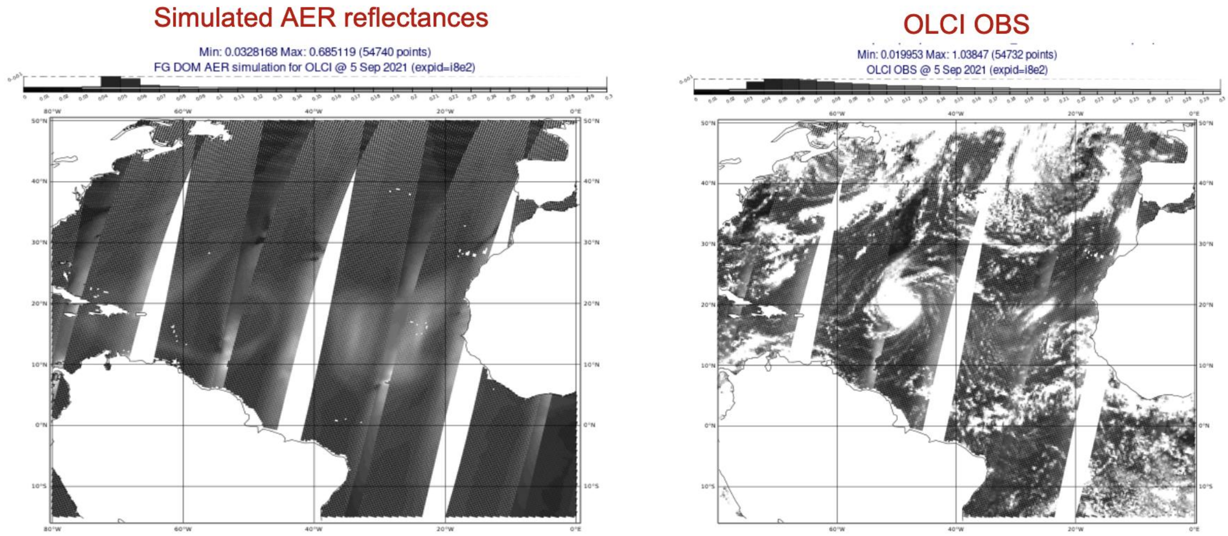


Figure 5. Simulated aerosol only reflectances using DOM for OLCI in CY48R1 on 5 Sep 2021 in the vicinity of hurricane Larry (left) and OLCI observations (right).

6 Preparations for RTTOV v14

The interface to RTTOV v14.0 has changed significantly compared to RTTOV v13.x. One of the major changes in v14.0 is bringing the capabilities of the RTTOV-SCATT model (for microwave scattering) inside RTTOV and thus enabling scattering across the full spectrum within RTTOV itself. The wider aim, to be developed further in future releases, is to eliminate spectral distinctions wherever possible to provide better spectral consistency. RTTOV v14.0 is the first step in this process. Since this already involves substantial updates, RTTOV developers decided to make further user interface changes at the same time to improve clarity and consistency in the interface, and with the aim of having smaller interface updates with future major releases.

Some user interface changes are relatively superficial, and involve changes in variable, derived type, and subroutine names, and/or subroutine argument order. However, other changes are more fundamental, primarily the way the atmospheric profile is represented, how cloud/hydrometeor scattering simulations are run, and the input/output of surface emissivity and reflectance.

Implementation of RTTOV-14 in CY49R1 (to be used in CY50R1) is progressing well. Note that MFASIS-Aerosols will only be available in RTTOV-14. Work focuses now on operationally assimilated instruments and will expand to the visible once the former is complete.

The current status of implementation and testing is as follows:

- The microwave all-sky and clear-sky route for
  - monitoring isimplemented and currently being tested
  - assimilation is implemented and under final debugging
- The infrared clear-sky route for
  - monitoring is implemented and under final debugging
  - assimilation implementation is undergoing
- The visible will follow the infrared route

RTTOV v14 profiles use level quantities while RTTOV v13 profiles use layer quantities. Therefore, the transformation from level to layer quantities in satrad/rttov/ifs/rttov_ec.F90 implemented for RTTOV v13 will not be necessary for v14. At this stage, we do not anticipate that porting the RTTOV interfaces with aerosol fields described section 4 to RTTOV v14 would involve any additional major changes.

We have been informed by DWD that a MFASIS-Aerosol version suitable for monitoring only will be made available to us very soon, which is very timely with our developments and progress. MFASIS-Aerosol with the assimilation capability (tangent linear and adjoint modules) will follow in the coming months.

7 Conclusions and next steps

In this document we have set out a description of all the elements required to implement an observation operator for aerosol visible reflectance assimilation:

- The BUFR template for visible reflectances will facilitate the possibility of using a wider range of observations, either GEOS or LEO, operationally
- RTTOV v14 is a requirement to be able to use MFASIS-Aerosols and differences with RTTOV v13 have been understood
- The RTTOV interfaces with aerosol fields have been implemented in RTTOV v13 and the changes required to implement it them in RTTOV v14 have been anticipated
- Initial monitoring tests using DOM with RTTOV v13 are promising

The next immediate step will be to run a monitoring experiment with MFASIS-Aerosols (once the monitoring capability is available) and compare the simulated reflectances to DOM calculated reflectances based on RTTOV v14 and CY49R1.

Once the full MFASIS-Aerosols with assimilation capability is available and integrated in RTTOV v14, the first assimilation experiments could be run. At this stage, we could consider the following options:

- Use Level-2 cloud-cleared visible reflectances (eg. from VIIRS/MODIS) and simulate/assimilate them running MFASIS-Aerosols
- Use non cloud-cleared visible reflectances (eg. from GEOS, or OLCI) by applying a cloud-screening using O-B departures, and then simulate/assimilate them running MFASIS-Aerosols

For the time being only one wavelength is tested (0.64 microns). However other waverlenghts will also be included (0.86 microns for example) in order to discriminate better cloud versus aerosol features when using L1 reflectances and/or to extract some size information in the Level-2 cloud-cleared reflectances. In the future, it would be interesting to have an MFASIS version capable of simulating simultaneously cloud and aerosols, as we can do with DOM, rather than an MFASIS-Cloud and an MFASIS-Aerosols separate versions. In the meantime, and despite not being a linear problem, it would be interesting to test how the addition of reflectances simulated from three separate runs of MFASIS-Cloud and MFASIS-Aerosols and a clear-sky run (no clouds or aerosols) compare to the ones simulated with DOM in a passive experiment.

Document History

Version	Author(s)	Date	Changes
0.1	Samuel Quesada-Ruiz, Angela Benedetti	13 May 2024	Initial version
0.2	Samuel Quesada-Ruiz, Angela Benedetti	23 May 2024	Revised version including comments from the internal reviewers
1.0	Samuel Quesada-Ruiz, Angela Benedetti	23 May 2024	V1.0 issued

Internal Review History

Internal Reviewers	Date	Comments
Jeronimo Escribano	16-05-2024	
Yves-Marie Saint-Drenan	16-05-2024	