CAMS Service Evolution

D1.6 Delivery and report on Observation-Operator-Post-Processor (OOPP)

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1 Executive Summary

Aerosols play a crucial role in a multitude of atmospheric processes like chemistry, radiation balances and cloud formation and are harmful to human health. The wavelength dependent interactions between aerosols and radiation are quantified by column integrated bulk optical properties like aerosol optical depth (AOD), single scattering albedo (SSA) and asymmetry parameter as well as three dimensional diagnostics such as extinction and backscatter coefficients.

The ECMWF's Integrated Forecasting System (IFS) provides these diagnostics in the forecasting mode and assimilates satellite observed AODs in a reanalysis system. Based on modelled aerosol mass mixing ratios (MMR) the optical diagnostics are computed. This step can also be performed independently from the IFS model in a standalone offline post processor. Such a tool enables quick calculations because it avoids the necessity to calculate independent processes like transport and chemistry. As mentioned in CAMEO deliverable D1.4 currently, there are inconsistencies between aerosol optical properties used in various remote sensing algorithms (both for satellite and ground-based observations of aerosol optical diagnostics) and in the climate and chemical transport models such as IFS. Aerosols are represented with different optical properties, sizes, and modal distributions. To be able to quickly test the effect of the selected optical representations, an offline optical operator is a useful tool.

Such an offline optical post processor (OOPP) has been developed and is tested by ingestion of MMRs and 're-computation' of optical diagnostics that are subsequently compared to equivalent quantities directly downloaded from the Climate Data Store (CDS). The AOD, SSA and asymmetry parameters at 550 nm over Europe (latitude [0:73], longitude [-27:65]) were downloaded from the CDS for a single day (2024-01-01 00:00, 06:00, 12:00, 18:00) as these were created by a recent version of IFS (Cy48r1). The region was chosen such that computations can be performed with limited memory demand (8Gb). Spatiotemporal correlations between OOPP computed and downloaded optical diagnostics were respectively 0.999, 0.977 and 0.972 for the AOD, SSA and asymmetry parameter. Additional statistics are summarized Table 5. It is clear that correlation are nearly one, biases and nRMSEs are small, showing OOPP can accurately reproduce the aerosol optical diagnostic fields.

The core of OOPP is based on IFS code and any future developments in OOPP should be easily integrated back into the IFS model. A detailed description of OOPP can be found in this document. Users that simply want to start working with OOPP should follow the steps in Chapter 4.

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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 the atmospheric composition including aerosol concentrations.

As mentioned in CAMEO deliverable D1.4, currently, there are inconsistencies between aerosol optical properties used in various remote sensing algorithms (both for satellite and ground-based observations of aerosol optical diagnostics) and in the climate and chemical transport models such as IFS. Aerosols are represented with different optical properties, sizes and modal distributions. To be able to quickly test the effect of the selected optical representations an offline optical operator is a useful tool.

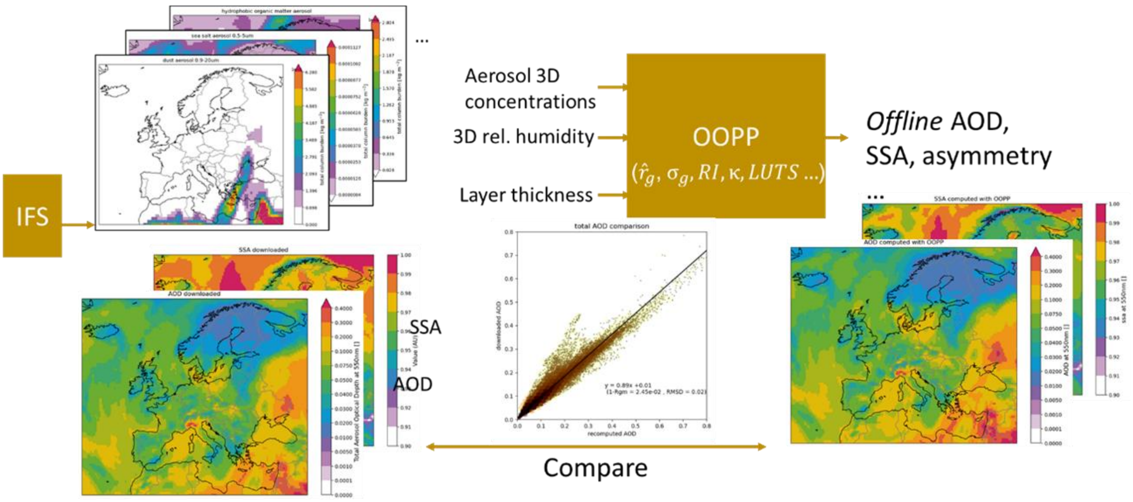

Figure 1 - Illustration of OOPP showing inputs and outputs.

Such an Optical Operator Post Processor named OOPP has been developed and is described in this document. The data flow of the operator is illustrated in Figure 1.This tool can be applied independently from the chemical transport model because only resulting concentrations are required to compute the optical diagnostics. In other words, the bulk optical properties of aerosols are assumed independent from the physical and chemical processes that govern their lives in the atmosphere.

These bulk optical properties are governed by Mie scattering. Mie scattering describes how electromagnetic waves interact with dielectric spheres. These interactions depend on the microscopic properties of the sphere, e.g., complex refractive index and size, and the wavelength of the radiation. In most chemical transport models including IFS, representative bulk mass extinction coefficients, single scattering albedos and asymmetry parameters are determined and used to translate mass mixing ratios into optical diagnostics (AOD, single scatter albedo, etc). This bases on assumptions on size distributions and dielectric properties for each aerosol species.

2.2 Scope of this deliverable

2.2.1 Objectives of this deliverables

This deliverable gives a technical description of OOPP, including guidelines on how to acquire and use the postprocessor. Initial tests performed with OOPP are presented.

2.2.2 Work performed in this deliverable

- The IFS model (v48r1) was used as a backbone for OOPP.
- The routines and modules required to calculate optical diagnostics from aerosol mass mixing ratios were incorporated into OOPP.
- Around this core functionality, tooling is developed
    - to download data from the CDS, load data in OOPP,
    - translate OOPP data in arrays expected by the IFS routines,
    - execute these routines,
    - write out optical diagnostics as netCDF files
    - and finally plot results.

2.2.3 Deviations and counter measures

No deviations have been encountered.

2.2.4 CAMEO Project Partners:

ECMWF	EUROPEAN CENTRE FOR MEDIUM-RANGE WEATHER FORECASTS
Met Norway	METEOROLOGISK INSTITUTT
BSC	BARCELONA SUPERCOMPUTING CENTER-CENTRO NACIONAL DE SUPERCOMPUTACION
KNMI	KONINKLIJK NEDERLANDS METEOROLOGISCH INSTITUUT
SMHI	SVERIGES METEOROLOGISKA OCH HYDROLOGISKA INSTITUT
BIRA-IASB	INSTITUT ROYAL D'AERONOMIE SPATIALEDE BELGIQUE
HYGEOS	HYGEOS SARL
FMI	ILMATIETEEN LAITOS
DLR	DEUTSCHES ZENTRUM FUR LUFT - UND RAUMFAHRT EV
ARMINES	ASSOCIATION POUR LA RECHERCHE ET LE DEVELOPPEMENT DES METHODES ET PROCESSUS INDUSTRIELS
CNRS	CENTRE NATIONAL DE LA RECHERCHE SCIENTIFIQUE CNRS
GRASP-SAS	GENERALIZED RETRIEVAL OF ATMOSPHERE AND SURFACE PROPERTIES EN ABREGE GRASP
CU	UNIVERZITA KARLOVA

CEA	COMMISSARIAT A L ENERGIE ATOMIQUE ET AUX ENERGIES ALTERNATIVES
MF	METEO-FRANCE
TNO	NEDERLANDSE ORGANISATIE VOOR TOEGEPAST NATUURWETENSCHAPPELIJK ONDERZOEK TNO
INERIS	INSTITUT NATIONAL DE L ENVIRONNEMENT INDUSTRIEL ET DES RISQUES - INERIS
IOS-PIB	INSTYTUT OCHRONY SRODOWISKA - PANSTWOWY INSTYTUT BADAWCZY
FZJ	FORSCHUNGSZENTRUM JULICH GMBH
AU	AARHUS UNIVERSITET
ENEA	AGENZIA NAZIONALE PER LE NUOVE TECNOLOGIE, L'ENERGIA E LO SVILUPPO ECONOMICO SOSTENIBILE

3 Aerosol optics in the CAMS IFS model (v48r1)

3.1 Physical description

In this document, the aerosols as presented in IFS version v48r1 will be described in more detail. With respect to earlier IFS versions the calculation of optical diagnostics from the aerosols mass mixing ratios has not changed conceptually, but some major changes in aerosol speciation and properties (e.g. the introduction of secondary organic aerosols) have occurred (summarized in Table 1).

In IFS v48r1, the forecast simulations produce mass mixing ratios for 16 aerosol tracers. There are three dust and sea salt tracers, two black carbon, nitrate, secondary organic and primary organic tracers and a single sulphate and ammonium tracer. Currently OOPP only supports computation of aerosol diagnostics in same way as the IFS v48r1.

It should be noted that the changes in the processes and resolution generally change the aerosol concentration but not necessarily change the optical representation.

Table 1 – Selection of changes made in the IFS system between the different model versions with respect to model resolution and aerosol representation. The links point to ECMWF Support pages which have a complete overview and more detailed information.

Cycle	**Changes in aerosol and optical properties**	levels	**CAMS Global FC and AN**	**CAMS Reanalysis (EAC4)**
48r1	Atmospheric composition • Two new secondary organic aerosol tracers (anthropogenic and biogenic) • Revision of aerosol optical properties (dust , brown carbon) • Improved secondary inorganic aerosol simulation	L137	2023-06-27 onwards N256 (~0.35/~40 km)	-
47r3	Atmospheric composition • Updated aerosol dry deposition • Updated aerosol wet deposition		2021-10-12 onwards N256 (~0.35/~40 km)	-
…				
46r1	Atmospheric composition • Biomass-burning injection heights from GFAS, and updated diurnal cycle. • Anthropogenic SOA production updated with a diurnal cycle and regionally-varying ratio to CO emissions. • New online dust emission scheme.	L137	2019-07-19 onwards N256 (~0.35/~40 km)	-

Cycle	Changes in aerosol and optical properties	levels	CAMS Global FC and AN	CAMS Reanalysis (EAC4)
	• Sea-salt production over freshwater lakes eliminated. • New nitrate and ammonium aerosol species, coupled to the gas-phase nitrogen chemistry. • Sulfur species (SO_2 and SO_4) coupled between chemistry and aerosol schemes			
42r1	EAC4 IFS model description	L60		2003 onwards N128

3.2 Mie calculations

Table 2 lists the relevant parameters for each of the chemical species:

- Dust
- Sea salt
- Sulphate
- Ammonium
- Nitrate
- Black Carbon
- Organic matter (primary and secondary, organic and anthropogenic)

It should be noted that the descriptions in Table 2 are used for the computation of aerosol optical properties with Mie code separately and not used internally in OOPP. The bulk optical properties:

- mass extinction coefficient (Ext)
- single scattering albedo (ω)
- asymmetry parameter (g)
- Lidar ratio (S)

are computed with a standard code for Mie scattering based on (Wiscombe, 1980). These descriptions have been used to fill the look-up-table (LUT) that is used in OOPP. Hence it is crucial to know how the aerosols are represented even though they are not calculated within OOPP.

For the hydrophilic species, the optical properties change with the relative humidity due to the hygroscopic growth of the water soluble component. The values are taken from (Tang & Munkelwitz, 1994) for sea salt, from (Tang et al., 1997) for sulphate and ammonium, from (Chin et al., 2002) for BC, from (Svenningsson et al., 2006) for nitrate and from the OPAC (Optical Properties of Aerosols and Clouds) database (Hess et al., 1998) for organic matter (OM). The refractive index (*m*) and density (*ρ*) are based on volume weighting following:

$$m\big(r(RH)\big) = \frac{V_{water}m_{water} + V_{aer}m_{aer}}{V_{water} + V_{aer}} = \frac{(\frac{4}{3}\pi r^3 - \frac{4}{3}\pi {r_{dry}}^3)m_{water} + \frac{4}{3}\pi {r_{dry}}^3 m_{aer}}{\frac{4}{3}\pi r^3}$$

$$m(r(RH)) = \frac{(r^3 - r_{dry}{}^3)m_{water} + r_{dry}{}^3 m_{aer}}{r^3} = m_{water} + \frac{r_{dry}{}^3}{r^3}(m_{aer} - m_{water})$$

The growth with respect to the default mass mixing ratios for each of the aerosol species in the IFS model as function of relative humidity (RH) is summarized in Table 3.

Table 2 - The chemical species and their properties relevant for the Mie calculations used in the IFS model.

Aerosol specie (tracers)	Refractive index reference	Size distribution(s)
Dust (3: fine, coarse, supercoarse)	-200-1000nm: a simulation using an experimental version of IFS-COMPO that represents twelve dust mineralogical species is used. -1000 to 3000 nm range values provided by (Balkanski et al., 2007) for dust with 0.9% hematite. -3000-10000 nm, values from (Di Biagio et al., 2017) have been used.	Bins: (0.03-0.55, 0.55-0.9, 0.9-20)
Sea salt (3: fine, coarse, supercoarse)	Optical Properties of Aerosols and Clouds (OPAC) database ((Hess et al., 1998).	Bins (80% RH): (0.03-0.5, 0.5-5.0, 5.0.-20)
Black carbon (2: hydrophobic and hydrophilic)	OPAC database with a value at 500nm of 1.75 for the real part and 0.45i for the imaginary part.	(0.0118, 2.0) (r, sigma)
Organic matter (2: hydrophobic and hydrophilic)	Only primary organic matter is included (different from older IFS versions) with properties from (Brown et al., 2018)	(0.09 1.6) (r, sigma)
Sulphate	The refractive index is taken from the Global Aerosol Climatology Project (GACP, https://gacp.giss.nasa.gov/datasets/) and it is representative of dry ammonium sulphate.	(0.0355,2.0) (r, sigma)
Ammonium	Ammonium uses similar refractive index as for sulphate.	(0.0355,2.0) (r, sigma)
Nitrate (2: fine and coarse)	nitrate from gas/particle partitioning (fine mode nitrate) has spectrally constant value of 1.611+0i. Nitrate from heterogeneous reactions coarse mode nitrate uses a spectrally constant value of 1.51 +0.001i.	(0.0355,2.0) & (1.992, 2.0) (r, sigma)
Secondary organic aerosols (2: anthropogenic and biogenic)	A spectrally constant value of 1.5+0.01i for anthropogenic SOA and 1.4+0.01i for biogenic SOA, following (Moise et al., 2015).	(0.09,1.6) (r, sigma)

Table 3 - Hygroscopic growth of aerosols w.r.t. the default mass mixing ratios; the default representation of the sea salt MMR is at 80% relative humidity (RH).

RH (%)	0	10	20	30	40	50	60	70	80	85	90	95

Sulphate	1	1	1	1	1.169	1.22	1.282	1.363	1.485	1.581	1.732	2.085
Sea salt	0.503	0.503	0.503	0.503	0.724	0.782	0.838	0.905	1	1.072	1.188	1.447
Organic matter	1	1	1	1	1	1.05	1.1	1.15	1.2	1.25	1.3	1.4
Nitrate	1	1.1	1.2	1.3	1.35	1.4	1.5	1.6	1.7	1.8	2	2.2
SOA	1	1	1	1	1	1.2	1.3	1.4	1.5	1.6	1.7	1.8

Based on these assumptions the bulk mass extinction coefficients, asymmetry parameters (the cosine-weighted average phase function), single scattering albedo and lidar ratios (the ratio of the extinction-to-backscatter coefficient) are calculated and stored as a look-up-table (LUT) in a netCDF file for each individual aerosol species (and at different relative humidities for the hydrophilic aerosols). An example of data stored in the netCDF file is shown in Figure 6.

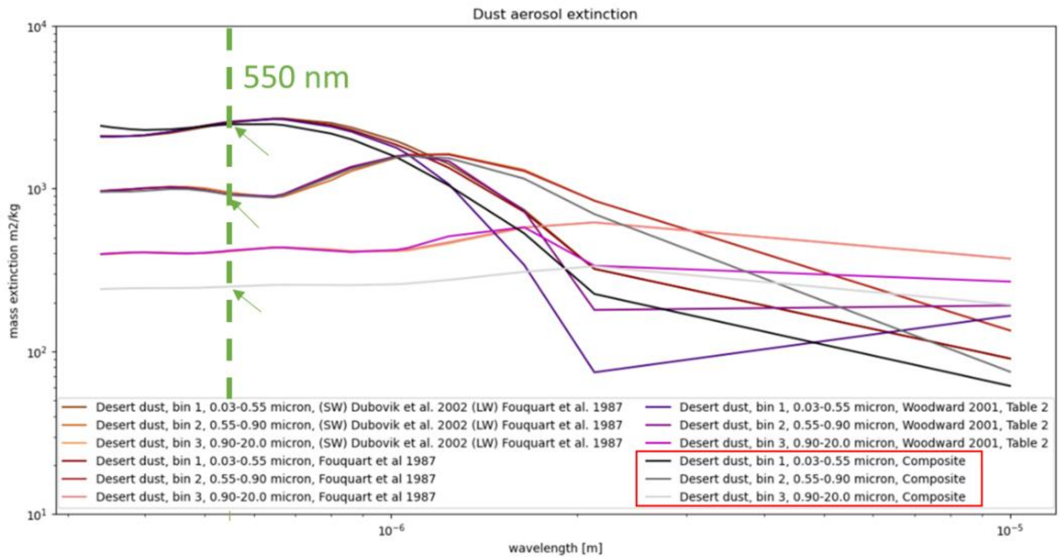

Figure 2 - The mass extinction coefficient of mineral dust in the three size bins in the IFS model as function of wavelength. Multiple representations of dust are available in the look-up-table (LUT) as shown by the various curves.

3.3 Aerosol diagnostic calculations

The mass extinction coefficient for all aerosol species (collected from the LUTs) is multiplied with air density and the mass mixing ratio to obtain model level extinctions for each aerosol species, which is then summed over all species to obtain total aerosol extinction at each model level. Vertical integration is then carried out to compute total AOD at a requested selection of the 20 available wavelengths, i.e., at 340 nm, 355 nm, 380 nm, 400 nm, 440 nm, 469 nm, 500 nm, 532 nm, 555 nm, 645 nm, 670 nm, 800 nm, 858 nm, 865 nm, 1020 nm, 1064 nm, 1240 nm, 1640 nm, 2130 nm and 10000 nm.

The aerosol absorption is computed for each species and each model level by multiplying the simulated aerosol extinction by (1 - SSA) where SSA is the single scattering albedo computed offline by the Mie code and stored in the LUT. Similarly to AOD, this is then summed over species and integrated over the vertical to provide absorption AOD (AAOD) at the requested selection of the 20 available wavelengths.The calculations are given below.

The *aerosol masses* in each model cell per cell area in [kg/m^2] are

$$ml_{aer}(lon, lat, lev) = MMR_{aer}(lon, lat, lev)\ \Delta P(lon, lat, lev)/R_g$$

Dimensional analysis $\frac{kg}{m^2} = \left[\frac{kg}{kg}\right]\left[\frac{kg}{ms^2}\right]\left[\frac{s^2}{m}\right]$

where R_g is the gravity constant, .e.g. 9.80665 m/s^2, ΔP is the pressure difference between the top and bottom of the grid cell as determined from the half level pressures, and MMR_{aer} is the mass mixing ratio of the aerosol.

The unitless *aerosol specific AOD* contribution per layer ΔAOD_{aer} is calculated as:

$$\Delta AOD_{aer}(lon, lat, lev) = ml_{aer}(lon, lat, lev)\ Ext_{aer}(RH),$$

Dimensional analysis $[-] = \left[\frac{kg}{m^2}\right]\left[\frac{m^2}{kg}\right]$

where $Ext_{aer}(RH)$ is the aerosol specific mass extinction coefficient that is dependent on relative humidity for the hydrophilic aerosols.

The *aerosol specific extinction* per layer is computed with

$$K_{aer}(lon, lat, lev) = MMR_{aer}(lon, lat, lev) Ext_{aer}(RH) \rho(lon, lat, lev),$$

Dimensional analysis $\frac{1}{m} = \left[\frac{kg}{kg}\right]\left[\frac{m^2}{kg}\right]\left[\frac{kg}{m^3}\right]$

where $\rho(lon, lat, lev)$ is the air density.

These quantities are subsequently integrated to calculate the *total extinction* and *total AOD*:

$$AOD(lon, lat) = \sum_{aer}\sum_{lev} \Delta AOD_{aer}(lon, lat, lev)$$

$$K(lon, lat, lev) = \sum_{aer} K_{aer}(lon, lat, lev).$$

The *single scattering albedo (SSA)* of the atmosphere is computed in a similar way. Note that the column integrated SSA is weighted with the extinction per layer because in layers where more aerosols are present, the SSA will contribute more to the average SSA of the column:

$$\omega(lon, lat) = \frac{1}{AOD(lon, lat)} \sum_{aer}\sum_{lev}\ \Delta AOD_{aer}(lon, lat, lev)\ \ \omega_{aer}(RH).$$

The *asymmetry parameter* of the atmosphere is computed again in a similar way. Note that the column integrated asymmetry is with weighted both with the extinction and the SSA per layer because where more aerosols are scattering light, the asymmetry parameter will contribute more to the average asymmetry of the column:

$$g(lon, lat) = \frac{1}{AOD(lon, lat)} \frac{1}{\omega(lon, lat)} \sum_{aer}\sum_{lev} \Delta AOD_{aer}(lon, lat, lev)\ \ \omega_{aer}(RH)\ g(RH).$$

3.4 Technical implementation of the calculation of optical diagnostics

OOPP is a standalone tool that can be used to download aerosol mass mixing ratios, compute atmospheric optical diagnostics and plot the model outputs.
In the original IFS code, the aerosol optical diagnostics are computed in the routine **AER_BDGT_MSS** called from **AER_PHY3**. This is shown in Figure 3. In OOPP, these routines are translated into **AER_BDGT_MSS_OOPP** and **AER_PHY3_OOPP** (where irrelevant parts of the code are removed or commented and some required additions are made). This is represented as yellow blocks in Figure 3.

As shown in Figure 3, the aerosol optical diagnostics are computed using precomputed aerosol optical properties, which have been calculated offline using Mie code for each aerosol described in Table 2 for 20 different wavelengths. These aerosol optical properties are available in a netCDF file. The netCDF file is read by IFS as part of the radiation scheme upon initialization. In OOPP, this has been replaced by a new specific input routine. Selected values from the file are stored in IFS arrays that serve as a look-up-table. Together with the downloaded mass mixing ratio of each aerosol tracer, air density and relative humidity, the look-up-table is used to compute the extinction per aerosol species.

In its current version, OOPP comes with the same capabilities as the IFS model (and is based on the same source code) This means that it is possible to calculate the AOD, SSA, ASY and Lidar ratio for all aerosol species as well as the contributions from the individual aerosol tracers to the diagnostics. Internally, 3D extinction coefficients are computed as mentioned in section 3.4. Without large adaptations OOPP can hence also produce extinction profiles to compare with for example Raman lidar signals.

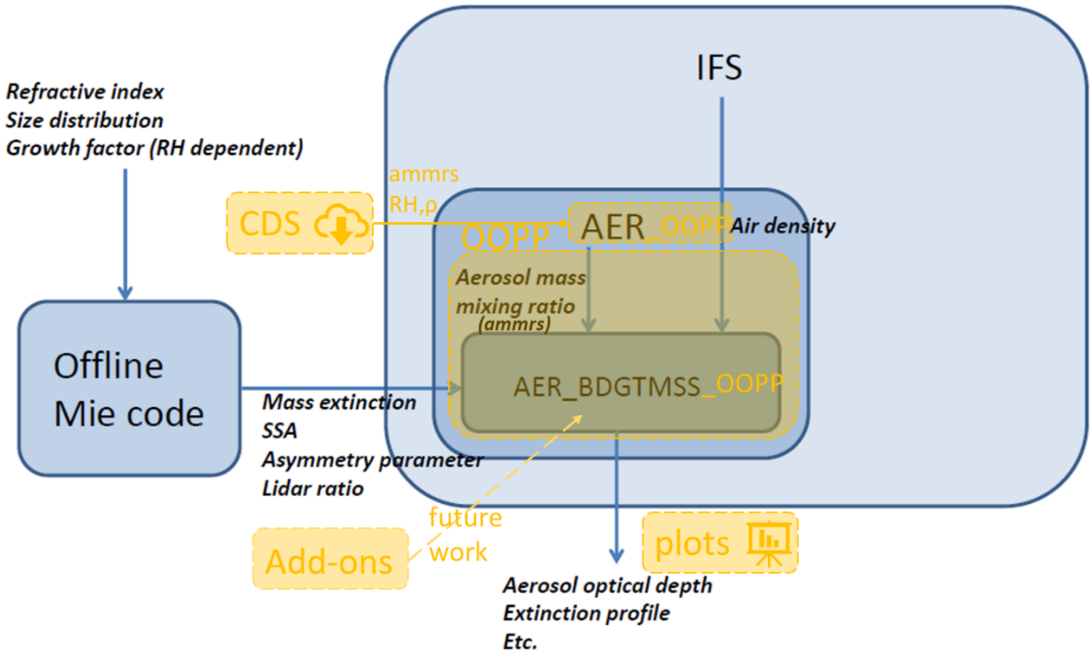

Figure 3 - Schematic showing how the aerosol optical diagnostics are computed, using aerosol optical properties that are computed offline with a Mie code, loaded and stored as arrays in the IFS. The yellow parts are incorporated in OOPP, eventually after modification of the original IFS codes. OOPP receives the aerosol mass mixing ratios not from IFS but uses archived fields that are for example downloaded from CDS.

OOPP comes with a downloading tool to collect data from the Climate Data Store (CDS). By default all relevant aerosol data are downloaded from a given data stream, such as “cams-global-reanalysis-eac4” for IFS reanalysis data or “cams-global-atmospheric-composition-forecasts" for forecast data. Next to the aerosol concentrations, the 3d pressure field is required to convert mass mixing ratios into mass concentrations or integrated aerosol masses. From the climate data store, only the surface pressure can be downloaded but using the hybrid coefficient definition of the IFS model the three dimensional pressure distribution can be computed. Hence, there is a capability integrated in the downloading tool to append the surface pressure with the hybrid coefficients as a preprocessor step to generate input required by OOPP.

4 Getting and running OOPP

4.1 Source code package

OOPP can be downloaded from a GIT server hosted by TNO:

ci.tno.nl/gitlab/cams/oopp

Currently, access is restricted to CAMEO project partners. An account is required to access the server. The authors can be contacted to obtain an account.

4.2 Documentation

OOPP comes with documentation describing how the tool is used. Compile the documentation using (requires Python's Sphinx package):

```
make docu
```

Figure 4 shows the main page of the OOPP documentation. New users are recommended to follow the "*Tutorial"* pages for a first introduction of the package and the configuration.

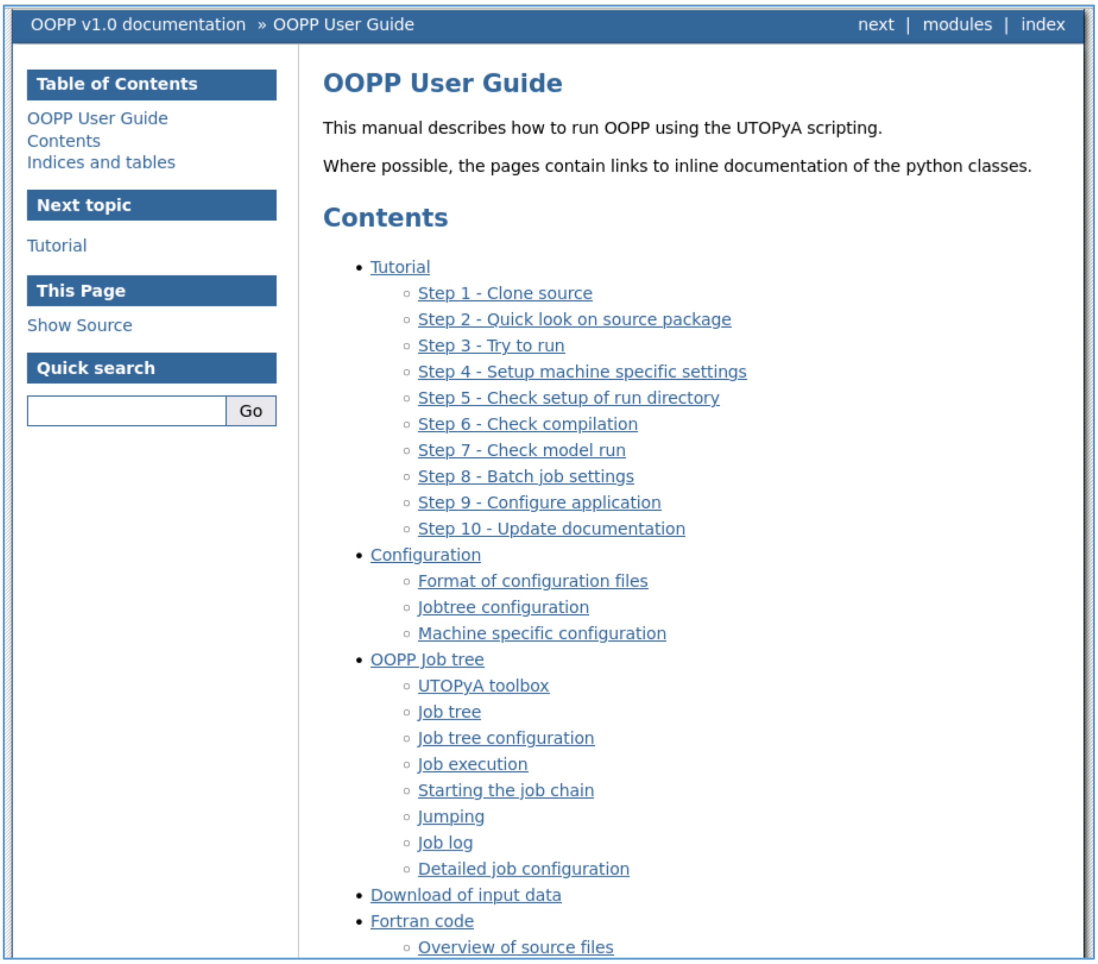

Figure 4 - Main page of OOPP package documentation.

4.3 Package content

After downloading the source, a folder structure shown in Figure 5 will be created.

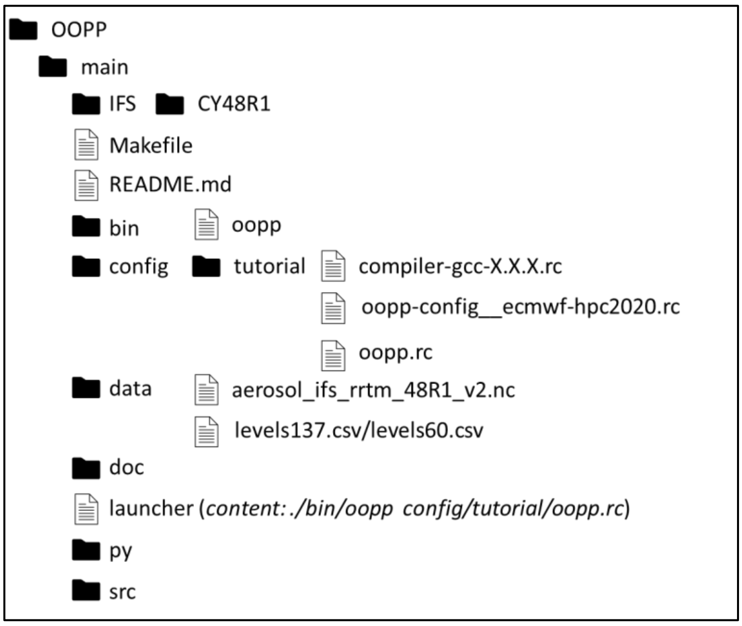

Figure 5 – File structure of OOPP.

In OOPP, configuration parameters can be set in the rc-files (for example found in `config/tutorial`) that govern the way in which the tool is applied. Generally the settings that need to be adjusted by the user are specified in *oopp.rc.* In this file, the user can specify which tasks OOPP will perform under the job-tree elements flag. A selection of *copy, download, build, run* and *post* jobs is specified to tell if OOPP needs to *copy* the required code and data into a user defined location, *download* data from the CDS, *build* the tool from the source code, *run* the tool and make figures based on the *post* job.

In this rc-file, other settings are provided by the user that for example specify the region and period of interest, the temporal resolution, the aerosols that need to be considered, the required output etc. The rc-file is rather self-explanatory and each flag has associated comments to describe which settings are specified by it. Two more rc-files are used to specify system specific setting, such as the Fortran compiler flags in `compiler-gcc-X.X.X.rc`, and the machine settings (e.g., `oopp-config__ecmwf-hpc2020.rc`), which specifies the environment modules need to be loaded on the platform where OOPP is running.

In the `data` folder, the level definition data is available that is appended to the surface pressure in order to be able to compute 3d pressure distributions. This folder furthermore contains the precomputed aerosol optical properties calculated with Mie code.

The original routines taken from the IFS model (v48r1) required to compute optical diagnostics can be found in the folder `IFS/CY48R1`. Together with the OOPP source code found under `src`, these Fortran files perform the actual computations.

In the `py` folder the Python scripts and libraries needed to run an OOPP application can be found.

5 Application

The calculation of optical properties by the OOPP package has been verified by comparison with optical properties archived from IFS simulations.

5.1 Description of the experiment

Atmospheric composition data from the IFS forecasting system was downloaded for testing. An arbitrary day, for which data from IFS v48r1 is available, was selected to test the performance of OOPP. The region (over Europe) was chosen such that computations can be performed with limited memory demand (8Gb).

- 2024-01-01 forecast data [at '00:00','06:00', '12:00','18:00']
- 137 model levels
- Regular grid; latitude [0:0.4:73] and longitude [-27:0.6:65], regridded with respect to the native model grid[1]
- All aerosol fields[2], required meteorological fields and AOD550 (total, dust, sea salt, sulphate, black carbon, etc)

OOPP computations were performed with the downloaded fields and compared to downloaded equivalents. This means for each aerosol chemical species, the contribution to the AOD was calculated at 550 nm and compared to the downloaded AODs (per time instance).

5.2 Metrics

The downloaded and with OOPP computed optical diagnostics are compared by multiple statistical metrics. The normalized root mean square error (nRMSE) is the RMSE divided by the mean of the downloaded metric. The geometric mean correlation coefficient is computed to assess how well observed spatial and temporal variability in concentrations is captured by the model. Lastly, the bias is a measure of structural over- or underestimations in the recomputed field. Formulas to compute the metrics of interest are as follows (overbars denote mean quantities):

Mean bias:
$$\mathrm{Bias}=\frac{1}{\mathrm{N}}\sum\left(\mathrm{C}_{\mathrm{model}}-\mathrm{C}_{\mathrm{observation}}\right) \quad (1)$$

Root mean square error:
$$\mathrm{nRMSE}=\sqrt{\sum\left(\mathrm{C}_{\mathrm{model}}-\mathrm{C}_{\mathrm{observation}}\right)^2}\Big/\overline{\mathrm{C}_{\mathrm{observation}}} \quad (2)$$

Geometric mean correlation:
$$\mathrm{R}^2=\left(\frac{\sum\left(\mathrm{C}_{\mathrm{model}}-\overline{\mathrm{C}_{\mathrm{model}}}\right)\left(\mathrm{C}_{\mathrm{observation}}-\overline{\mathrm{C}_{\mathrm{observation}}}\right)}{\sqrt{\sum\left(\mathrm{C}_{\mathrm{model}}-\overline{\mathrm{C}_{\mathrm{model}}}\right)^2\sum\left(\mathrm{C}_{\mathrm{observation}}-\overline{\mathrm{C}_{\mathrm{observation}}}\right)^2}}\right)^2 \quad (3)$$

In these equations C stands for the (modelled or observed) atmospheric optical diagnostic (generally unitless) and N for the total number of data points considered.

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[1]CAMS Global atmospheric composition forecasts data has a resolution of approximately 40 km x 40 km (approximately 0.35 degrees). The data are archived either as spectral coefficients with a triangular truncation of T511 or on a reduced Gaussian grid with a resolution of N256. These grids are so called "linear grids", sometimes referred to as TL511.

[2]https://confluence.ecmwf.int/display/CKB/CAMS%3A+Global+atmospheric+composition+forecast+data+documentation

5.3 Comparison of OOPP and IFS on interpolated grid

For the individual aerosols, the AOD contributions are available from the CDS. The comparison with equivalents computed with OOPP are shown in Figure 6. Because the recomputed AODs closely match (in space and time) with the downloaded AODs leading to correlation close to one, we report 1-R. To calculate this, all datapoints in space and time were compared for the selected diagnostics. Table 5 summarizes the results that are also added to the scatter plots in Figure 6. Table 5 clearly reveals that correlations are high (particularly for the hydrophobic dust, black carbon and OM aerosols) and the biases and nRMSE are low.

For the hydrophilic aerosols, the nRMSE is relatively high. For the total AOD, the single scattering albedo and the asymmetry parameter, the diagnostic results are shown in Figure 7 and summarized in Table 5. The spread in the single scattering albedo and the asymmetry parameter are larger than in the total AOD but nonetheless correlations are high (higher than 0.97) and nRMSEs and biases are low (maximally 0.065 in absolute terms).

Table 4 - Statistical metrics describing the equivalence between AOD contributions from each aerosol downloaded from the CDS and computed with OOPP.

AOD550	1-R	Bias	nRMSE
Sea salt	2.6e-3	-0.0018	0.10
Sulphate	5.5e-3	-0.00073	0.15
Organic matter (OM)	9.12e-5	4.9e-5	0.034
Secondary OM	2.9e-3	-0.0017	0.20
Dust	1.2e-6	-9.3e-6	0.003
Black Carbon	2.3e-6	-1.4e-6	0.0028
Nitrate	9.4e-3	-0.00012	0.26
Ammonium	5.0e-3	-7.9e-5	0.14

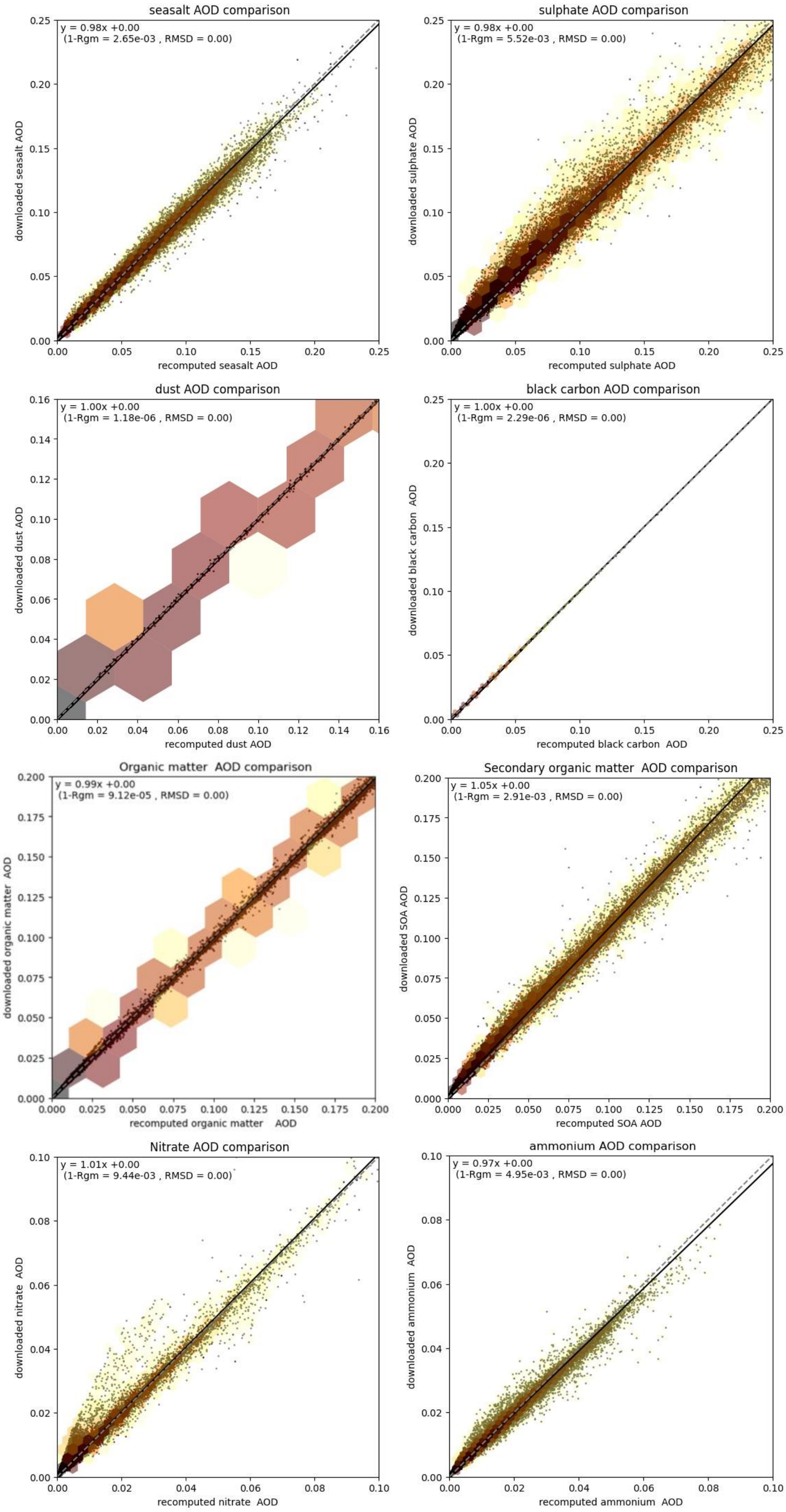

Figure 6 - Scatterplots showing the AOD per aerosol specie computed with OOPP (x-axis) vs downloaded (y-axis). From left to right and top to bottom: the AOD contribution from sea salt, sulphate, dust, black carbon, organic matter, secondary organic matter, nitrate and ammonium aerosols are shown. The hexagons show the sample density withing their boundaries, with darker colours if more samples are in their area.

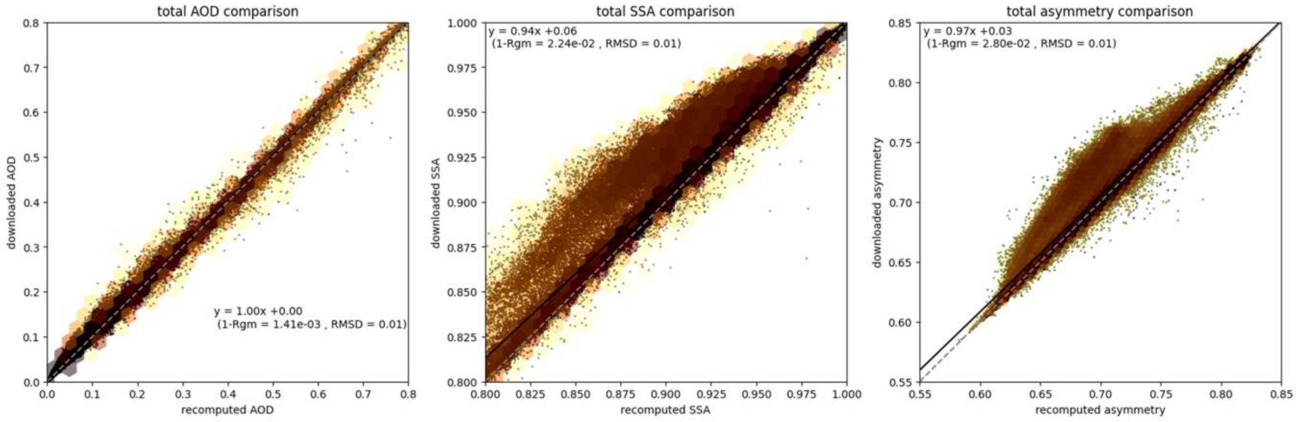

Figure 7 - Scatterplots showing the total AOD, single scatter albedo and asymmetry parameter computed with OOPP (x-axis) vs the downloaded equivalent (y-axis).

Table 5 - Statistical metrics describing the equivalence between optical diagnostics downloaded from the CDS and computed with OOPP.

	1-R	Bias	nRMSE
AOD 550 nm	1.4e-3	0.0028	0.061
SSA 550 nm	2.3e-2	-0.0059	0.014
Asymmetry 550 nm	2.8e-2	-0.0046	0.014

6 Conclusion

OOPP is able to compute optical diagnostics that accurately match with the optical diagnostics produced by the IFS model (correlations >0.97 and nRMSE<0.065). With OOPP, the inputs (aerosol mass mixing ratios, surface pressure, temperature and specific humidity) can be downloaded from the CDS and (aerosol specific contributions to) the AODs, the SSA, asymmetry parameter and lidar ratio can be computed. For aerosols influenced by water uptake, OOPP is less accurate than for hydrophobic aerosols.

For the hydrophilic aerosols, the single scattering albedo and asymmetry parameter deviations between the values computed with OOPP and downloaded from the CDS are evidently present. For these quantities, non-linear effects with respect to relative humidity (through water uptake) are assumed to cause the differences. The downloaded fields are gridded to a regular cartesian longitude-latitude grid that differs from the native IFS grids (The data is for example archived on a reduced Gaussian grid with a resolution of N256). If these diagnostics are computed on the native IFS model grid, the values will differ from the values computed based on resampled inputs. This hypothesis should be tested by performing a similar experiment directly on data at the native IFS grid.

7 Discussion

The current OOPP could be extended with other elements of IFS that could be used to validation optical properties. For example, the IFS code in AER BDGTMSS also calls AER_LIDSIM to simulate observations available from lidar stations, and this could be useful extension to OOPP too. Likewise extensions to deal with other bulk aerosol optical properties (e.g. other LUTs) can be easily implemented in OOPP and quickly tested. This also holds for the introduction of a more smoothened water uptake scheme (now a step function) through for example linear interpolation. This type of quick tests are possible with OOPP as well as the computation of optical diagnostics at other wavelengths (based on the 20 available options) not available from the CDS.

Capabilities to compare with measurement data (e.g., satellite and AERONET AOD data, but also other measured quantities like backscatter and extinction profiles) should be developed to make effects of aforementioned description changes quantifiable. Furthermore, incorporation of the calculation of extinction profiles, depolarisation ratios and backscatter profiles would allow more detailed comparisons with measurements. The AOD is a metric in which a lot of information is lost, because of vertical integration and its insensitivity to aerosol species. Taking into account more measurement data gives access to additional information (for example on vertical profile based on extinction and backscatter and on dust loading based on depolarization ratio) that can be used to test the optical representation in the LUTs and improve OOPP and subsequently the IFS model and its reanalysis capabilities.

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