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Preparing an extension of RTTOV-DOM for application to ICON-ART aerosol


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 <p>EUMETSAT NWP SAF NUMERICAL WEATHER PREDICTION</p>	<p>Preparing an extension of RTTOV-DOM for application to ICON-ART aerosols</p>	<p>Doc ID : NWPSAF-DWD-VS-059 Version : 1.0 Date : 14/04/2022</p>
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2 Introduction

This report summarizes the results of a collaboration between Lukas Muser (KIT) and Christina Köpken-Watts, Christina Stumpf, and Leonhard Scheck during a visiting scientist mission at DWD between 17 January and 14 April 2022. The aim of this work was to extend the radiative transfer model RTTOV for the simulation of satellite radiances based on ICON-ART (ICOsahedral Nonhydrostatic - Aerosols and Reactive Trace gases) model output. The current implementation and available optical parameters in RTTOV allow already the simulation of radiances based on CAMS aerosol fields, but need adaptations for ICON-ART aerosol fields taking the differences between the aerosol modelling approaches in CAMS and ICON-ART into account.

3 Motivation and Approach

Additionally to extending the application range for RTTOV simulations to other aerosol models, this work is also motivated by the development of a fast approximation, the MFASIS-aerosol approach, of the computationally demanding RTTOV-DOM (Discrete Ordinates Method) simulations in the visible range. This ongoing development follows requests from CAMS and ICON-ART model users in the CDOP-3 period. As a first step, simplifications in the vertical representation of aerosol distributions and their impact on the accuracy of reflectance have been investigated using CAMS aerosol profiles. In order to develop the MFASIS approach in a generalized and efficient way, similar work is needed involving ICON-ART aerosol profiles with a corresponding simulation of reflectance using RTTOV-DOM.

ICON-ART (Rieger et al., 2015; Weimer et al., 2017; Schröter et al., 2018) uses a different, and in some ways more complex, representation of aerosol than CAMS. This includes more and different aerosol classes and an explicit simulation of particle size distributions. The interaction of prognostic aerosols with radiation is considered in the radiative transfer calculation in ICON-ART (Gasch et al., 2017, Rieger et al. 2017). Mineral dust can be treated as non-spherical particles (Hoshyaripour et al., 2019). Furthermore, ICON-ART can allow for chemical ageing which modifies the optical properties of the aerosol particles over the course of the integration (Muser et al., 2020). The underlying model of the CAMS data is the IFS-AER model, developed and operated by ECMWF. Within this report the word “CAMS” is used synonymously for the underlying IFS-AER model.

In order to extend RTTOV, the first step was to compare the basic assumptions of the aerosol modelling approaches in the CAMS and ICON-ART models. A short summary of this comparison is given in Section 4. This was followed by extending the RTTOV code to allow for a consistent processing of the ICON-ART aerosols. The work plan foresaw the implementation of two example species for which different approaches are followed in ICON-ART for describing their optical properties. The choice was made to implement two species with a treatment of optical properties similar to CAMS (soot and sea salt) and one species where descriptions differ (mineral dust). The technical steps during implementation are described in Section 5, which is also detailing a suggested approach for a further extension to allow for the dependency of optical properties on the aerosol particle radii. Section 6 presents examples of modelled radiances and reflectances based on the implemented ICON-ART optical properties and Section 7 provides a short summary and outlook.

4 Comparison of aerosol representation in ART and CAMS

Atmospheric aerosols are of different origin and have varying chemical composition and properties. Additionally, aerosols exist in a great range of particle sizes, stretching over several orders of magnitude. To account for this variety, transport models represent a certain number of different aerosol species and in order to reflect the different particle sizes, the models need to resolve the particle size distribution to some degree. Typically, there exist two types of modelling approaches for representing aerosol size distributions, sectional and modal. A sectional model uses multiple discrete size bins to resolve the particle size distribution with particles in one size bin having a fixed particle diameter. A modal aerosol model approximates the particle size distribution with a log-normal distribution. Thus, one mode represents a range of different particle sizes. Arbitrary examples of such size distributions in both modelling approaches are displayed in Figure 1 and Figure 2 for illustration.

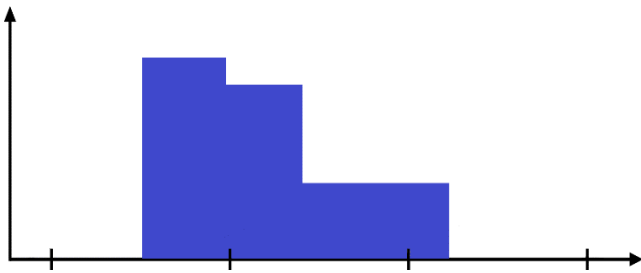


Figure 1 Example of a sectional aerosol description. The graph illustrates the number concentration of particles as a function of particle radius.

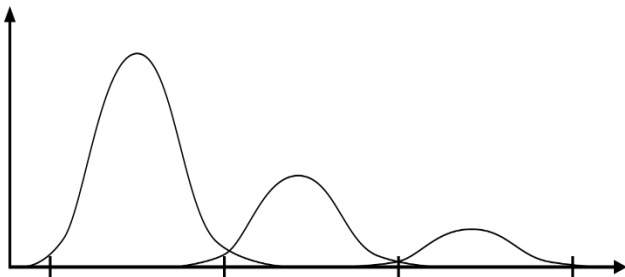


Figure 2 Example of a modal aerosol description. The graph illustrates the number concentration of particles as a function of particle radius.

Particles in the CAMS model are represented by a sectional, i.e. binned, size distribution. In contrast to that, ICON-ART uses a modal description.

There are also differences between the prognostic variables that are used in CAMS and ICON-ART which have implications for the interpretation of the model output. In CAMS, one size bin is represented by one prognostic variable, the mass mixing ratio. Consequently, particles in one size bin are assumed to have the same diameter. In ICON-ART, typically a two-moment approach is used. This means, the model solves transport equations for two prognostic variables, the mass mixing ratio and the number concentration. Under the assumption of a constant standard deviation for the log-normal distribution, the particle median diameter can be derived from mass mixing ratio and number concentration. Consequently, the particle diameter for a given mode can vary in ICON-ART during runtime.

Table 1 lists typical aerosol species that can be simulated by CAMS and ICON-ART. The table also lists the number of bins and modes that resolve the particle size distribution of one species in CAMS

Table 1 Different aerosol species in CAMS and ICON-ART. The numbers in brackets give the number of bins and modes that resolve the particle size distribution in CAMS and ICON-ART, respectively. The greyed out species are available in the corresponding model for transport, but no optical coefficients are available for RTTOV applications (yet).

CAMS		ICON-ART	
Soot	(1 bin)	Soot	(1 mode)
Sea salt	(3 bins)	Sea salt	(3 modes)
Mineral dust	(3 bins)	Mineral dust	(3 modes)
Sulfate	(1 bin)		
Organic matter	(1 bin)		
Ammonium	(1 bin)	Pollen	
Nitrate	(2 bins)	Volcanic ash	
		9 AERODYN modes	

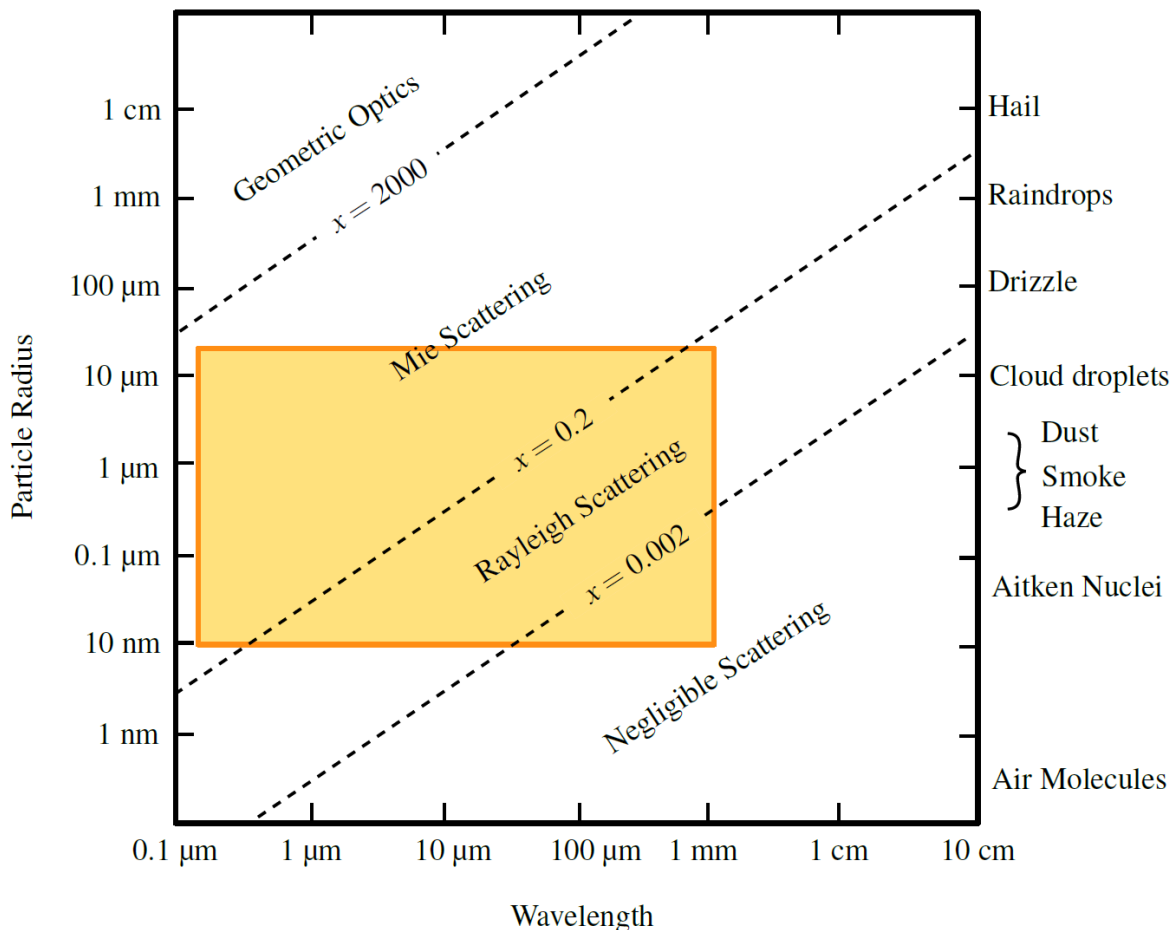


Figure 3 Scattering regimes depending on wavelength and particle size. Highlighted by the orange box is a range of typical wavelengths and atmospheric particle sizes. The variable x denotes the size parameter. Adapted from Petty (2006).

and ICON-ART, respectively. Additionally to the aerosols of a given type, like soot, sea salt, mineral dust, pollen, volcanic ash, ICON-ART allows the formation of internally mixed particles, e.g., volcanic ash coated by sulfate and water. Muser et al. (2020) give details on these nine so-called AERODYN modes treated in the AERODYN module of ICON-ART. Consequently, not only the particle median diameter of a mode can change, but also its chemical composition. As the treatment of such flexible modes with varying compositions in radiative transport models is rather complex, they are listed in Table 1 for the sake of completeness and as an outlook for future extensions. Also, note that not all

of the available CAMS aerosols are currently included in RTTOV, as optical properties are not yet available for ammonium and nitrate.

The interaction of aerosol with solar and terrestrial radiation can be considered both, online during the numerical simulation in aerosol transport models and offline in radiative transport models or forward operators such as RTTOV. In both cases, the optical properties of the particles are needed. These optical properties are the scattering phase function, the extinction, the scattering, and the absorption coefficient. There exist several methods to determine these properties, e.g., Mie calculations or T-Matrix calculations. All methods need information about the particle size distribution and the particle composition as well as an assumption on the particle shape.

Figure 3 shows the influence of different particle sizes on the scattering regimes. These regimes are separated by the non-dimensional size parameter

$$x = \frac{2\pi r_p}{\lambda}$$

in which r_p denotes the particle radius and λ the wavelength. Highlighted by the orange box is a range of typical atmospheric aerosol sizes and typical atmospheric wavelengths.

As the Mie theory (Mie 1908) holds for both, the Mie and Rayleigh scattering regime, so called Mie calculations allow the computation of the necessary optical properties. However, the Mie theory is based on the assumption of spherical particles. This spherical assumption is typically not true for solid particles such as mineral dust or volcanic ash. Other approaches like T-Matrix calculations are specifically designed for non-spherical particles.

Figure 4 shows the influence of the non-sphericity of particles on the scattering phase function at two different wavelengths. Especially in the backscatter region, hence, at scattering angles close to 180°, the difference between spherical and ellipsoidal particles is largest. This results in substantially less backscattering for non-spherical particles.

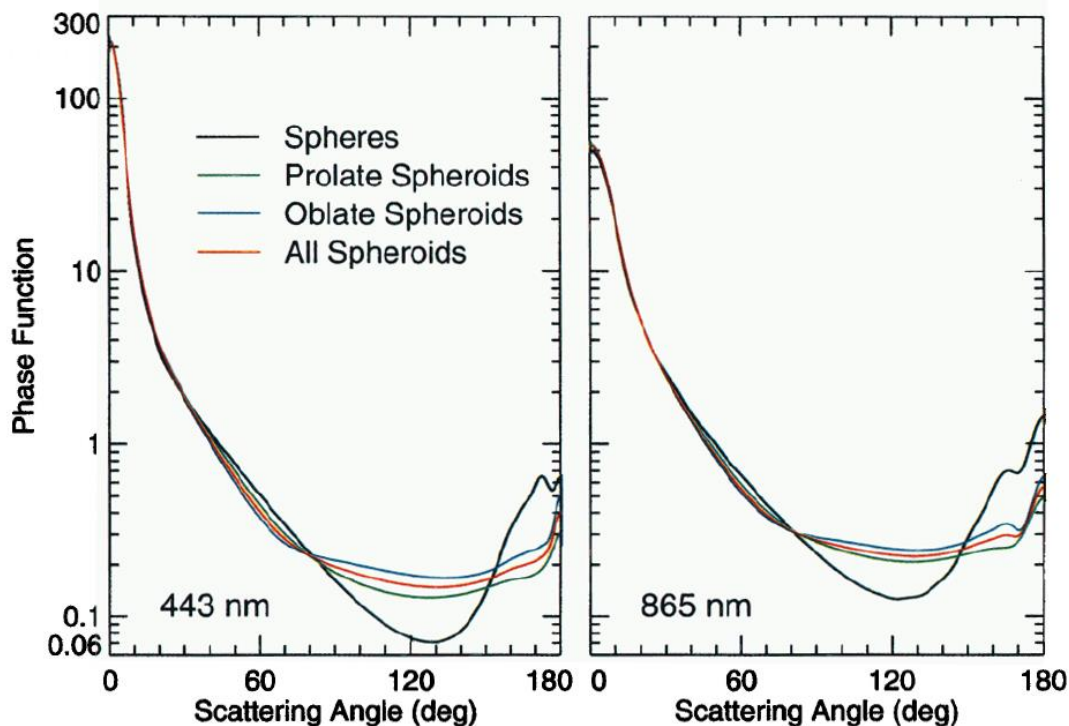


Figure 4 Scattering phase functions for polydisperse spheroidal and spherical particles at two wavelengths. Particles with different aspect ratios form the spheroid population. Figure from Mishchenko et al. (1997).


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Table 2 Method for CAMS and ICON-ART particles to derive optical properties

CAMS		ICON-ART	
Soot	Mie Calculations	Soot	Mie Calculations
Sea salt	Mie Calculations	Sea salt	Mie Calculations
Mineral dust	Mie Calculations	Mineral dust	Meng et al. (2010)
Sulfate	Mie Calculations		
Organic matter	Mie Calculations		

The optical properties of particles in CAMS and ICON-ART are mostly derived from Mie calculations, as summarized in Table 2. Only the optical properties of mineral dust in ICON-ART are based on the data from Meng et al. (2010). Meng et al. (2010) applied several methods, such as T-Matrix calculations and geometric optics, to compile a dataset for tri-axial ellipsoidal mineral dust particles. The optical properties, as they are used online in CAMS and ICON-ART, are also used within RTTOV to ensure consistency between the numerical model and the forward operator.

As illustrated in Figure 3, the particle size significantly influences the interaction of radiation with particles. This is why the particle size distribution of aerosols needs to be taken into account for Mie calculations and also for exploiting the Meng et al. (2010) database. Although CAMS uses a sectional aerosol model, for the calculation of the optical properties with Mie theory a log-normal distribution is used. However, the particle size distribution is only evaluated between the diameter limits of the corresponding size bin. In practice, the log-normal distribution is discretized in small radius bins for which Mie calculations are performed or the Meng database is exploited. Finally, the weighted average of all discrete values is computed to determine the optical properties for the size bin or mode in CAMS or ICON-ART, respectively. These log-normal distributions are defined by the values listed in Table 3. Please note that in ICON-ART always one log-normal distribution is used per mode. For CAMS optical properties of sea salt, two log-normal distributions are superposed to determine the optical properties for all three size bins. The optical properties of the three mineral dust size bins in CAMS are determined based on only one log-normal distribution. Also, the median radius r_{med} in Table 3 is defined with respect to the number concentration. However, for ICON-ART mineral dust the median diameter $r_{med,3}$ is formulated with respect to the third moment of the size distribution, which can be related to the mass mixing ratio. Knowing the standard deviation of the log-normal distribution $r_{med,3}$ can easily be converted into r_{med} which is also given for ICON-ART in Table 3.

Table 3 Median radii r_{med} with respect to number concentration and standard deviation σ of log-normal distribution that describes the particle size distribution for the determination of the optical properties. All radii are given in μm .

	CAMS		ICON-ART	
	r_{med}	σ	r_{med}	σ
Soot	0.0118	2.0	0.595	1.41
Sea salt	0.1992	1.9	0.1	1.9
“	1.992	2.0	1.0	2.0
“	-	-	6.0	1.7
Mineral dust	0.29	2.0	0.322 ($r_{med,3}= 0.75$)	1.7
“	-	-	1.727 ($r_{med,3}= 3.35$)	1.6
“	-	-	4.336 ($r_{med,3}= 7.1$)	1.5
Sulfate	0.0355	2.0	-	-
Organic matter	0.021	2.24	-	-

The way how particles interact with radiation depends to a large extent on their chemical composition. A quantity that describes this behaviour is the complex refractive index. It is a material property and it is typically available from databases compiled in lab studies. The real part of the refractive index gives information about the phase velocity of the electromagnetic wave in the medium. The imaginary part indicates the rate of absorption. For optical properties of aerosols in CAMS and ICON-ART the refractive indices are taken from the databases listed in Table 4. The values of the refractive indices as they are used for CAMS and ICON-ART aerosol are displayed in Figure 5. The two top panels display the values used for soot aerosol. So far, there are almost no studies about the refractive index of soot aerosol from biomass burning events. Especially, data is missing over a wider range of wavelengths. For this reason, in CAMS only one constant value is used. In ICON-ART the real part is assumed to be constant, but two different values are assumed for the imaginary part.

For sea salt aerosol (Figure 5, middle panels), CAMS allows a dependence of the refractive index on the relative humidity and the grey lines in Figure 5 illustrate this behaviour. In ICON-ART, however, only one refractive index value at a relative humidity of 70% is used.

For mineral dust (Figure 5, bottom panels), a recent comprehensive study by di Biagio et al. (2019) exists and their result is also depicted in Figure 5 along with the values used in CAMS and ICON-ART. For ICON-ART mineral dust, it is planned to switch to the di Biagio et al. (2019) database in the near future.

The particle density is needed for the conversion between number concentration and mass mixing ratio which can be done in RTTOV. The particle densities assumed in CAMS and ICON-ART are listed in Table 5.

Table 4 Database for refractive indices.

	CAMS	ICON-ART
Soot		HITRAN
Sea salt	OPAC	HITRAN
Mineral dust	Woodward (2001)	Gasch (2016)
Sulfate	Lacis (2001, GACP)	-
Organic matter	WASO+, OPAC INSO+, SOOT	-

Table 5 Density of particles in $g\ cm^{-3}$. Organic matter in CAMS is a mixture of three species with different densities.

	CAMS	ICON-ART
Soot	1	1.7
Sea salt	2.438	1.25
Mineral dust	2.61	2.65
Sulfate	1.76	-
Organic matter	1.; 2.; 1.8	-

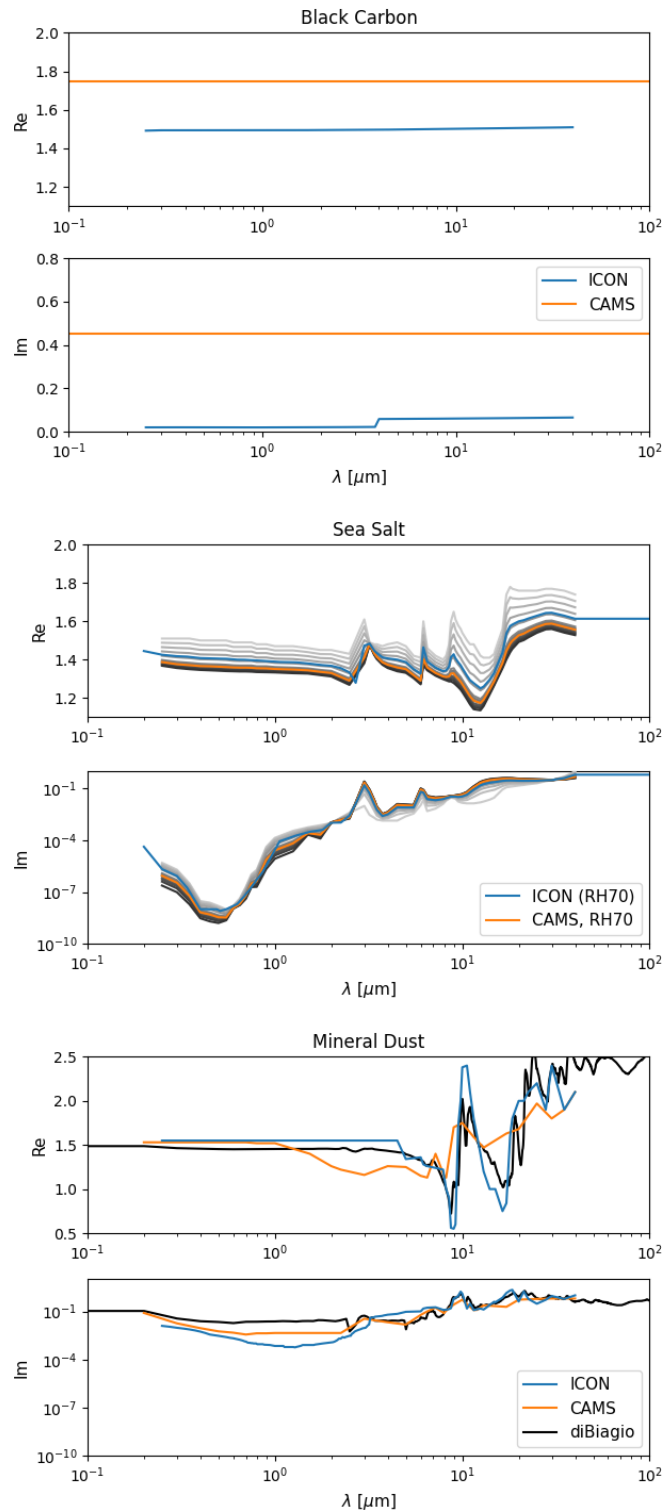


Figure 5 Complex refractive indices as a function of wavelength for soot, sea salt, and mineral dust as used for ICON-ART and CAMS aerosols. Note that CAMS sea salt optical properties are computed at 12 different relative humidity levels, hence, the grey curves indicate different relative humidity levels. The brightest and the darkest one represent 0% RH and 95% RH, respectively. For mineral dust, recent measurements by di Biagio et al. (2019) are indicated in black.

5 Technical Implementations

5.1 In RTTOV

The extension of the RTTOV capabilities done during the visiting scientist work have been added in the development framework of the software using the git repository, so that the extension is available for the official future development lines. The extension has been added for both RTTOV v13.2 and the v14 development code. The implementation in v13.2 will make the ICON-ART simulations available in the near future; while the preparation in v14 will allow adding further functionality with respect to varying particle radii and their influence on the optical properties (see section 5.3).

The following briefly describes the added functionality:

RTTOV needs information specifying the optical properties of the different aerosol types and their dependencies, e.g., on wavelength (see also Section 4). These optical properties are pre-computed for the different satellite instruments, i.e., specific channel frequencies, and stored in ASCII files. For RTTOV v14 these optical properties are mainly the extinction coefficient, the single scattering albedo (ssa), the asymmetry parameter, and the phase function. In RTTOV v13, instead of the extinction coefficient, single scattering albedo, and asymmetry parameter, the absorption and scattering coefficients are stored. The units of the extinction, the scattering, and the absorption coefficient must be in $\text{km}^{-1} \text{cm}^3$ which is the extinction (or scattering or absorption) per distance in km^{-1} and per number of particles per volume in $\# \text{cm}^{-3}$. Special care has to be taken regarding the correct units of the coefficients in the ASCII file, as this can be a simple source of error. The single scattering albedo, the asymmetry parameter, and the phase function are dimensionless.

For ICON-ART, the corresponding Fortran program `rttov_mie_params_aer_icon.F90` has been developed, based on an existing program for CAMS (`rttov_mie_params_aer_cams.F90`) which uses Mie calculations based on the input of refractive indices for a certain spectral range. A subroutine for Mie calculations is available in RTTOV. For ICON-ART, the same Mie calculation subroutine is used to compute the optical properties of spherical particles like soot and sea-salt, using the ICON-ART specific input parameters. Additionally, for non-spherical particles like mineral dust, a new functionality has been added through reading the Meng et al. (2010) database.


The input parameters for the Mie calculations and the exploitation of the Meng database, i.e., the particle size distribution, the particle density, and the complex refractive indices, are made consistent with the assumptions used in the ICON-ART radiative transfer.

The optical properties provided allow aerosol affected RTTOV calculations for ICON-ART both in the visible and the infrared range (i.e., through RTTOV-DOM and the Chou scaling approach).

5.2 In RadSim

For easy application of RTTOV to ICON-ART model output, we have prepared RadSim for ICON GRIB files with aerosols. This development has been done in a currently separate code version which will be handed over to James Hocking, once the following remaining minor open issues are resolved.

- In the newest version of RadSim the pressure on model half levels is needed. For ICON-ART model fields this proved to be slightly unhandy, as this variable is not routinely stored in DWD databases. The pressure on model half levels can be determined, however, based on the pressure on full levels and the corresponding model layer height and the corresponding calculations will be added to the code.

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- So far, no GRIB paramId has yet been assigned to ICON-ART soot from biomass burning events. Therefore, in the mean time some manual GRIB file manipulation needs to be done in order to read in soot profiles in RadSim.

Table 6 lists the currently implemented ICON-ART aerosols in RadSim. Please note that some GRIB paramIds can differ between centres. This can make adjustments in the RadSim code necessary.

Table 6 GRIB shortName and paramId of ICON-ART aerosols.

	shortName	paramId
Soot	Not assigned yet!	Not assigned yet!
Sea salt mode 1	SEASA	503247
Sea salt mode 2	SEASB	503248
Sea salt mode 3	SEASC	503249
Mineral dust mode 1	DUSTA	503241
Mineral dust mode 2	DUSTB	503242
Mineral dust mode 3	DUSTC	503243

5.3 Suggested further extensions

ICON-ART, in contrast to CAMS, integrates two prognostic aerosol variables instead of one: the mass mixing ratio and the number concentration. Due to the nature of the log-normal distribution and under the assumption of a constant standard deviation, the size distribution median radius can be diagnosed from the two prognostic variables. This also implies that the median radius of the particle size distribution can change during model integration. This additional information can also be used for RTTOV applications and would enable a better consistency between the optical properties used in ICON-ART and RTTOV calculations. For this purpose, the optical properties must be available for variable particle diameters. A simple linear interpolation in lookup tables proved to be unsuitable for a sufficiently accurate description. Therefore, in ICON-ART this issue is solved with polynomial functions fitted to optical properties at different particle diameters.

It is suggested that a similar approach should be implemented into RTTOV v14 (which is prepared to allow for more flexibility w.r.t. aerosol optical properties) through the following steps:

- Addition of external routines deriving the polynomial fit and an extension of the ASCII optical properties files to contain the coefficients of the polynomials
 Current implementation in ICON-ART uses a polynomial of third order. The example is given for the extinction coefficient (EXT), with the median diameter d_{med} :

$$EXT = p_1 d_{med}^3 + p_2 d_{med}^2 + p_3 d_{med} + p_4$$

- Extension of the optical properties data structure and adjustment of I/O within RTTOV
- Input of the particle radii OR number concentration through the extended input profile structure. The particle median radius can be determined based on mass mixing ratio and number concentration, given a known standard deviation of the log-normal distribution.
- Implementation of the polynomials in RTTOV to derive optical properties as a function of particle radius

Open questions remain about how to deal with polynomials for the full phase function and its derivatives, i.e., Legendre coefficients and the bpr parameter.

6 Results for SEVIRI

To demonstrate the new implementation in RTTOV, results of the “pilot” version of RTTOV used within RadSim are displayed in this section. RTTOV calculations are performed for atmospheric profiles containing the aerosols black carbon, sea salt, and mineral dust. The vertical profiles are taken in this example from CAMS fields of 20 February 2021 at 12 UTC. Once the remaining issues in RadSim for ICON-ART GRIB files are resolved, similar calculations can be done for ICON-ART fields as well. The optical properties ASCII file using the ICON-ART optical properties has been pre-computed with the newly developed Fortran program described in section 5.1. RTTOV calculations have been done for all twelve SEVIRI channels. A selection of the results is displayed in this section.

Figure 6 shows the column integrated aerosol mass in the used profiles. Please note the different colour bar for the top panel of soot.

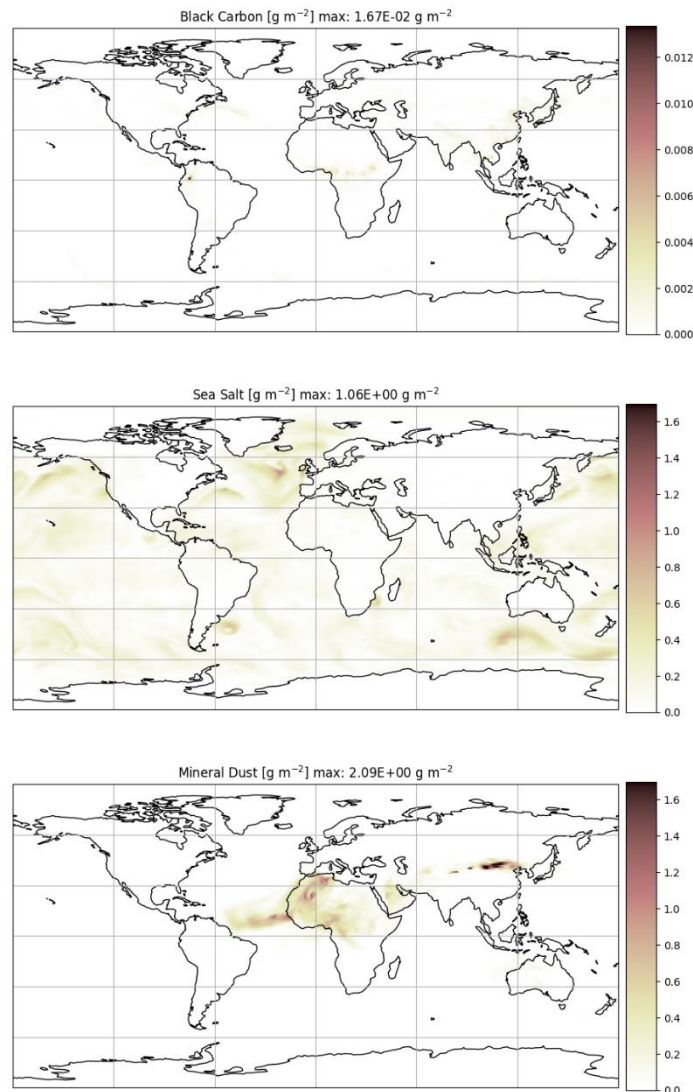


Figure 6 Column integrated aerosol load for soot (top), sea salt (middle), and mineral dust (bottom) in g m^{-2} .

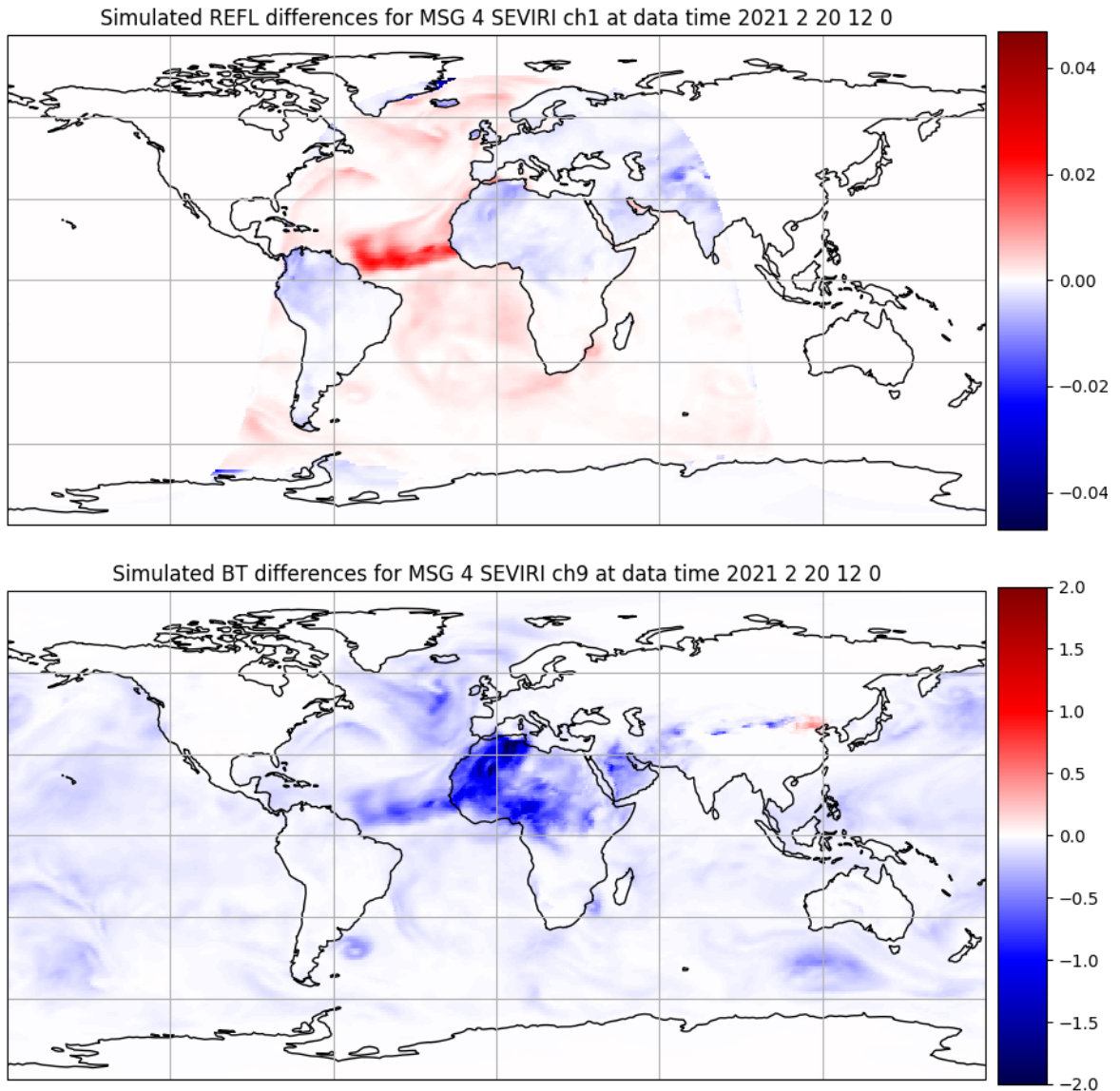


Figure 7 Difference in reflectance (top) for SEVIRI channel 1 at $0.64 \mu\text{m}$ and brightness temperature (bottom) for channel 9 at $10.8 \mu\text{m}$ between a simulation with aerosol – no aerosol. All three aerosol types, soot, sea salt, and mineral dust are included.

Figure 7 displays two difference plots between a simulation with aerosol minus a simulation without aerosol. The top panel shows the difference in reflectance for the SEVIRI channel 1 at $0.64 \mu\text{m}$. The presence of aerosol leads to higher reflectances over the ocean due to its low background albedo, while the aerosols over land and sea ice cause a decrease in reflectance values. The bottom panel shows the difference in brightness temperature for channel 9 at $10.8 \mu\text{m}$ for which the presence of aerosols leads to an overall reduction of the brightness temperature of mostly around -0.1 to -1 K with the largest reductions caused by the presence of mineral dust over the Sahara and the adjacent Atlantic ocean.

These contributions caused by the different aerosol types are visualized in Figure 8. Only the contributions due to mineral dust and sea salt are shown here, as soot is only present at rather low concentrations (see Figure 6).

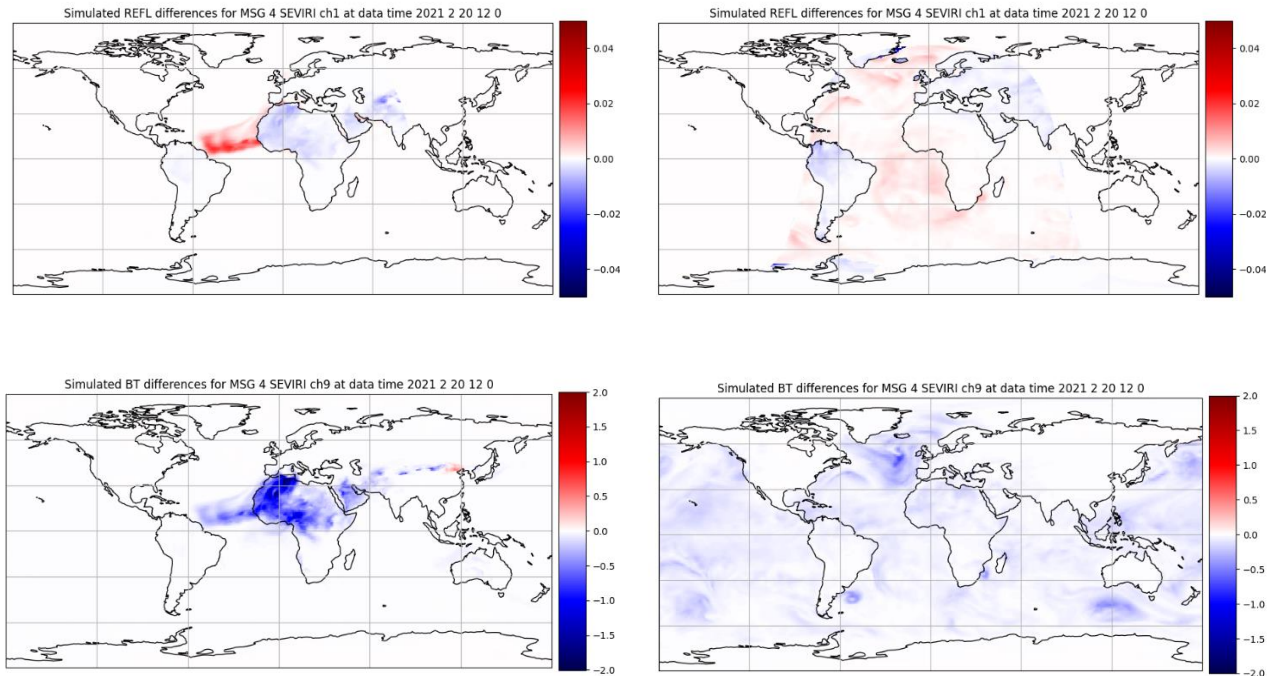


Figure 8 The left column displays the effects of mineral dust, the right column the effect of sea salt. The top row shows the difference in reflectance for the SEVIRI channel 1 at $0.64 \mu\text{m}$, the bottom row the difference in brightness temperature of channel 9 at $10.8 \mu\text{m}$.


7 Summary and Outlook

During this visiting scientist cooperation, a comparison of aerosol modelling approaches and the corresponding description of their optical properties in the CAMS and ICON-ART models has been made as a preparatory step for enabling RTTOV to simulate radiances based on ICON-ART aerosol profiles. An overview of this comparison is given in this report. RTTOV has then been extended for simulating the ICON-ART aerosol types soot, sea salt and mineral dust. The necessary calculations of aerosol optical properties consistent with the assumptions and description as used in ICON-ART were set up and the program made available within the RTTOV development git repositories for v13.2 and v14. In particular, the treatment of mineral dust as non-spherical particles has been enabled through implementing access to the Meng et al. (2010) database. This new feature offers additional potential to future RTTOV developments reaching beyond the ICON-ART applications.

Example and test simulations with RTTOV have been carried out using RadSim in an extended version allowing the input of ICON-ART aerosol fields. Simulations have been done for both the visible and infrared channels of SEVIRI and show a realistic behaviour of the simulated radiances and reflectances.

To further extend the ability of RTTOV for making use of variable aerosol particle radii information, an implementation approach and the corresponding necessary steps have been suggested using new capabilities prepared in RTTOV v14. However, some additional development is needed to also include a consistent description of the variation of the full phase function.

ICON-ART, especially the latest version with the AERODYN module, allows internally mixed particles, e.g., volcanic ash coated by sulfate and water. For RTTOV applications to these new

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aerosol species in ICON-ART, the variable particle composition should be considered for future extensions to RTTOV.

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