# NWP SAF

# RTTOV version 14
# Product Specification and Requirements Review

Version 1.2

15th October 2024

# RTTOV Version 14 Product Specification

This documentation was developed within the context of the EUMETSAT Satellite Application Facility on Numerical Weather Prediction (NWP SAF), under the Cooperation Agreement dated 7 September 2021, between EUMETSAT and the Met Office, UK, by one or more partners within the NWP SAF. The partners in the NWP SAF are the Met Office, ECMWF, DWD and Météo France.



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# 1. INTRODUCTION

This document defines the specification for Version 14 of RTTOV, in accordance with the requirements of the NWP SAF. The Product Specification describes the deliverable from the point of view of the user.

## 1.1 Reference documents

[RD-1] NWPSAF-MO-DS-039 RTTOV v13 Product Specification
[RD-2] RTTOV user survey 2022
[RD-3] RTTOV user survey 2017
[RD-4] RTTOV user survey 2014
[RD-5] NWPSAF-MO-PP-011 NWP SAF CDOP 4 Product Plan
[RD-6] NWPSAF-MO-VS-059 Improvement of the scattering parameterisation in RTTOV
[RD-7] NWPSAF-MO-UD-055 RTTOV v14 User guide
[RD-8] NWPSAF-MO-TV-050 RTTOV v14 Test Plan
[RD-9] NWPSAF-MO-UD-056 RTTOV v14 User interface changes

# 2. PURPOSE

RTTOV is a fast radiative transfer model for simulating top-of-atmosphere UV, visible, infrared (IR) and microwave (MW) clear-sky and aerosol- and/or hydrometeor-affected radiances for downward-viewing space-borne sensors. It is intended for use in NWP data assimilation systems, retrieval applications (for example 1DVAR), generating simulated imagery, reanalysis projects and instrument cal/val activities, among others. It consists of a forward model and associated tangent linear (TL), adjoint (AD) and Jacobian (K) models.

# 3. REQUIREMENTS

## 3.1 General considerations

Each RTTOV major release represents a development of the previous version. Existing functionality is only removed if it has been superseded by an improved alternative, if it was previously deprecated, or if it was originally introduced in an earlier minor release as a temporary option to maintain backwards compatibility. RTTOV v14 will therefore implement the majority of the RTTOV v13 Product Specification [RD-1], noting the features being removed described in section 3.6 below. Major releases also introduce significant updates to existing capabilities.

The following sections discuss the plans for major developments in RTTOV v14 with reference to user requirements. Broader developments in NWP, in radiative transfer modelling, and recommendations from groups such as the International TOVS Working Group (ITWG) on Radiative Transfer and Surface Properties are taken in account. User requirements for RTTOV are gathered by several methods:

- Discussions at conferences, particularly the International TOVS Study Conference (ITSC).
- Feedback from users via the NWP SAF Helpdesk.
- Feedback from users directly to RTTOV developers.
- User surveys (RTTOV surveys were made in 2022 [RD-2], 2017 [RD-3] and 2014 [RD-4]).

### 3.2 Ongoing development activities

Certain development activities listed in the Project Plan for RTTOV [RD-5] represent general improvements from which all (or many) users will benefit and as such are tacitly assumed to fulfil requirements of RTTOV users. These include:

- Keeping up to date with developments in spectroscopic databases and line-by-line models for training RTTOV gas optical depth coefficients.
- Developing the diverse profile set used for training RTTOV gas optical depth coefficients.
- Supporting new sensors or updating coefficients for existing sensors as new/modified spectral response function data become available. Note that for most sensors this only involves generating new coefficient files and that no code changes are required.
- Implementing new RTTOV functionality in the RTTOV GUI and the C++/Python wrapper. As new options and capabilities are added to RTTOV, these ancillary components of the software are updated to support them.
- Code optimisation to reduce run-times and memory requirements. These are focussed on the aspects of RTTOV which are known to be least efficient.

### 3.3 Core model changes

This section describes some fundamental changes to the core RTTOV model planned for RTTOV v14.

*Implementation of RTTOV-SCATT capabilities within RTTOV (i.e. unification of the models)*

RTTOV carries out clear-sky and UV/VIS/IR scattering simulations. RTTOV-SCATT is a separate radiative transfer model included in the RTTOV package that is used for MW scattering simulations. It calls RTTOV for the clear-sky radiance calculation but implements the delta-Eddington solver (not available in RTTOV), implements different cloud overlap options to RTTOV, and uses a different representation of hydrometeor inputs in the profile structure compared to that used by RTTOV for UV/VIS/IR scattering calculations (see below). There are other inconsistencies between RTTOV and RTTOV-SCATT in terms of internal calculations such as the unit conversions applied to hydrometeor concentrations among others.

From a scientific perspective, the separation of scattering between the two models is far from ideal. As NWP centres move increasingly towards all-sky assimilation across the whole spectrum, the spectral inconsistencies become important as they may lead to sub-optimal use of all-sky satellite observations. From a technical perspective, users interested in both MW scattering simulations, and clear-sky and/or UV/VIS/IR scattering simulations must interface to the two different models which creates additional complexity.

A significant goal of RTTOV v14 is to unify the two models so that MW scattering simulations can be done through the RTTOV interface in a very similar way to UV/VIS/IR scattering simulations. Users will only interface to one model and the spectral inconsistencies in the simulations will be very much reduced. RTTOV-SCATT will no longer exist.

The broad aim is to implement the existing science in RTTOV-SCATT within RTTOV. This includes the optical property interpolation, treatment of polarisation, the cloud overlap schemes, the delta-Eddington solver, and the radar solver. Code and capabilities will be shared across the spectrum where scientifically sensible. Thus, the delta-Eddington solver will be available for IR hydrometeor and aerosol simulations, and the DOM solver will be available for MW hydrometeor simulations (e.g. for off-line research purposes). All cloud overlap schemes will be available to all implemented solvers. The explicit optical property inputs available in RTTOV for UV/VIS/IR scattering simulations will be enabled for MW scattering simulations.

The 2022 RTTOV user survey [RD-2] shows there is strong support among users for this development, for example, nearly a quarter of all respondents indicated interest in this development.

The implementation of this update necessitates some other changes in RTTOV described below.

*Change in representation of atmosphere in input profiles*

Figure 1 shows the input profile structures in RTTOV v13 (and earlier), and that proposed for RTTOV v14. RTTOV v13 requires temperature, water vapour (and optionally other gases) to be supplied on vertical pressure levels. For VIS/IR scattering simulations, the cloud/aerosol inputs are provided for layers between the pressure levels. This is inconsistent with NWP models because they typically represent cloud/aerosol on the same vertical levels as temperature and gas concentrations. This means that users must adapt their profiles, in many cases omitting the top level of the cloud/aerosol profiles when passing them to RTTOV which represents a half-layer shift upwards compared to the NWP model field and thus leads to systematic biases in the RTTOV scattering simulations. By contrast RTTOV-SCATT uses the RTTOV pressure, temperature, and water vapour profiles, but in addition requires pressure half-levels interleaving the pressure levels, and the hydrometeor inputs are provided on the pressure levels. This is therefore consistent with the NWP model representation of the atmosphere but is obviously inconsistent with the cloud inputs for VIS/IR scattering simulations.

To unify RTTOV and RTTOV-SCATT, a unified representation of the atmosphere is required. The proposed profile structure for RTTOV v14 employs the pressure half-levels equivalent to those in RTTOV-SCATT, and all other inputs are provided on the pressure full-levels (or layers). This enables spectral consistency as well as consistency with the NWP model representation of the atmosphere.

The RTTOV gas optical depth parameterisation is carried out on a fixed set of atmospheric pressure levels. In early versions, users had to provide input profiles on these levels, and therefore it was necessary for RTTOV to accept the surface pressure (*p2m*) as an input independent of the pressure levels themselves. The radiative transfer equation is then integrated from the top of atmosphere down to *p2m*. Since RTTOV v9, an internal interpolator has been available that allows users to input profiles on arbitrary pressure levels. In general (and, in particular, for NWP, which is RTTOV's primary user domain) it is extremely beneficial, both scientifically and technically, to input profiles on the native NWP pressure levels rather than interpolating the profiles outside of RTTOV before input. NWP models typically have the surface at the bottom level of the input profile which makes the *p2m* input redundant in this case.

RTTOV-SCATT has never supported an arbitrary *p2m* and requires that the surface lies on the bottom pressure half-level. In addition, the flexible surface requires every solver in RTTOV to implement a special case for the partial layer that lies immediately above the surface, including potentially avoiding numerical issues when that partial layer is optically thin. This creates complexity in the code increasing the risk of bugs. It is a maintenance burden when modifying existing capabilities, and a development burden when implementing new solvers. Therefore, RTTOV v14 will no longer support the surface pressure as an independent input: the surface will implicitly lie on the bottom pressure half-level. As noted, for NWP users this has no implication because this is consistent with the NWP model representation of the atmosphere.

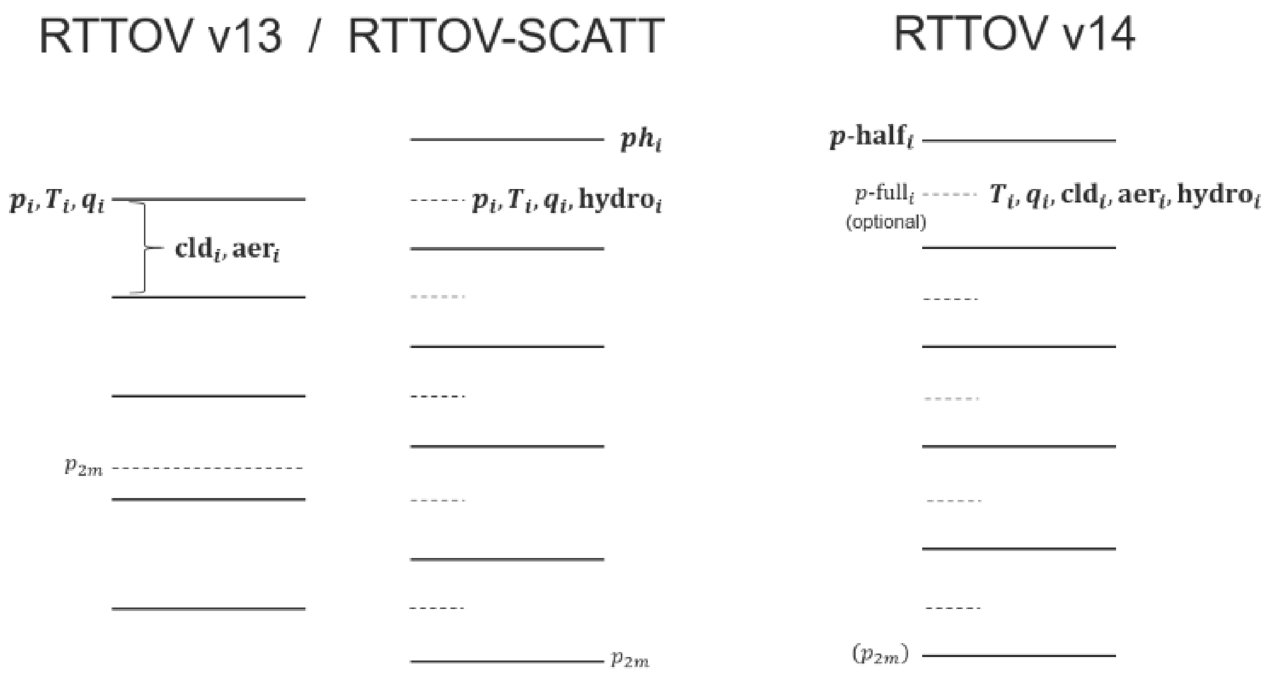


*Figure 1: the RTTOV / RTTOV-SCATT v13 and RTTOV v14 profile structures.*

This change is quite fundamental as it affects many aspects of RTTOV and as such it cannot be put on a switch in the code. Therefore, RTTOV v14 will be unable to replicate RTTOV v13 radiances. The new code will be thoroughly tested in data assimilation trials in the ECMWF IFS (Integrated Forecasting System).

The changes to the profile structure are a pre-requisite for unifying RTTOV and RTTOV-SCATT. They have been discussed within the RTTOV development team (who are aware of how RTTOV is used) and have been presented to knowledgeable RTTOV users, for example at the last two ITSC meetings. There has been no negative feedback on the proposal.

*Making VIS/IR hydrometeor optical properties more flexible*

When carrying out cloudy UV/VIS/IR simulations in RTTOV v13 (and earlier), users must choose one of two sets of cloud liquid water optical properties, and one of three sets of ice cloud optical properties. This is a very inflexible approach to the optical properties: no other types of hydrometeor could be represented (rain, snow, graupel, etc), and it makes it extremely difficult to create tools to enable users to make their own cloud optical property files for use with RTTOV.

This contrasts with UV/VIS/IR aerosol optical properties, which have always consisted of an arbitrary collection of particle types defined in the optical property files enabling the RTTOV team to supply users with different sets of optical properties, and to create a tool to allow users to make their own custom aerosol optical property files. Similarly, RTTOV v13 introduced a flexible MW hydrometeor implementation that works in the same way: the optical property file contains properties for an arbitrary collection of hydrometeors which may be used in any combination in the simulations.

The full (optimal) unification of RTTOV and RTTOV-SCATT involves changes to make the UV/VIS/IR cloud optical properties flexible in the same way. The same optical properties will be available in RTTOV v14 as in v13, but they can be used in any combination (no selection between sets of liquid and ice properties), and this will pave the way in future releases for additional hydrometeor types to be represented if desired, and for a user tool to be created to allow users to make their own optical properties. Furthermore, this also enables the possibility to create sets of hydrometeor optical properties across the full spectrum (UV/VIS/IR/MW) to further increase the spectral consistency in the simulations. This is therefore also considered a pre-requisite for the unification of the models, and users have expressed interest in this capability to the development team (for example, in discussions at workshops and conferences).

*Revised Fortran interface*

The changes described above involve some substantial changes to the interface to RTTOV. RTTOV v14.0 therefore provides a good opportunity to update other aspects of the user interface to improve clarity and consistency.

This will include the following changes:

Reorganisation of the structure containing the options with which users configure the simulations at run-time. Partly this will involve eliminating the spectrally-specific groups of options (i.e. no longer having IR- or MW-specific options). It will also involve renaming various options with obscure or inconsistent names (just one example is the *addaerosl* argument which enables aerosol simulations and is not a typo).

Various subroutines in the user interface (especially the routines for allocating/deallocating RTTOV data structures) take similar arguments, but the argument order is inconsistent between these routines. It is planned to improve the consistency and clarity of these interfaces.

Currently there are multiple surface emissivity and reflectance arguments to the core RTTOV routines (*rttov_direct/tl/ad/k*). These are optional, depending on the kind of simulation being done. However, emissivity and reflectance are related concepts. Furthermore, the “diffuse reflectance” that is used for downward emitted and scattered radiation has not been readily available as an output, nor is it available as an input for IR/MW simulations. RTTOV v14 will introduce a new data structure that contains all emissivity and reflectance and related inputs/outputs to RTTOV. It will also enable input/output of the diffuse reflectance in the same way as already implemented for emissivity and solar BRDF. This will simplify the interface for users and provides full control over the treatment of the surface by giving access to the diffuse reflectance for all channels. This is also considered a pre-requisite for the new mixed scenes capability described below.

Various other variables (for example in the profile structure) will benefit from being renamed to improve clarity.

Although there is no explicit user requirement for these changes, they constitute significant technical improvements to the code. User feedback indicates that new users find it challenging getting to grips with RTTOV and simplifying/clarifying the user interface can only help in this regard.

### 3.4 New capabilities

This section describes new capabilities that will be implemented in RTTOV v14.

*Mixed scenes capability*

RTTOV v13 assumes that the surface within the satellite footprint is homogenous and is assigned a single surface type: land, sea, or sea-ice. The surface type primarily affects the surface emissivity and reflectance that RTTOV computes (if requested by the user) for each channel. In practice it is common for satellite observations footprints to fall over coastline or over a combination of sea and sea-ice. In the latter situation particularly, it is not uncommon for NWP models to provide a sea-ice fraction and it is possible to retrieve the sea-ice fraction along with other profile variables within the 4DVar context. RTTOV v14 will provide the capability to specify multiple surface types for a given profile, each with an associated fractional coverage of the footprint. This will extend not only to the emissivities/reflectances, but the near-surface and skin variables in the profile structure, so that each surface will have a unique set of variables describing it.

This change is made technically much simpler (for both developers and users) by the refactoring of the emissivity and reflectance inputs and outputs described above (i.e., grouping them all within a single data structure), and hence that change is viewed as a pre-requisite for this new capability.

There are no explicit user requirements for this feature, but it can be noted that ECMWF are introducing a more restricted version of this in their RTTOV v13.2 operational implementation enabling the combination of water emissivities from the internal RTTOV sea surface models with user input land/sea-ice emissivities and associated fractional coverages of the land/sea-ice. It was decided that rather than implementing this more restricted approach in RTTOV v14, it would be better to introduce a fully generic capability for an arbitrary combination of different surface types. This will future-proof the code, for example, in case additional surface types are added in the future. It can also be noted that the Community Radiative Transfer Model (CRTM, see https://www.jcsda.org/jcsda-project-community-radiative-transfer-model) already implements something similar.

### 3.5 Enhancements of existing capabilities

This section describes planned developments of existing RTTOV v13 functionality to enhance these capabilities in RTTOV v14.

*MFASIS-NN*

The neural network (NN) version of the MFASIS fast visible cloud solver (Scheck, 2021), first introduced in RTTOV v13.2, has superseded the pre-existing look-up table (LUT) approach (Scheck *et al*, 2016). The NN version has comparable or improved accuracy than the LUT version, is faster, and is more extensible to channels that require additional inputs to accurately describe the radiative transfer problem, which is not feasible with the LUT approach due to the size of the tables. Similarly, the NN version can be extended to aerosols. The primary developments in MFASIS-NN for RTTOV v14.0 are code optimisation, and introduction of integrated water vapour input to the neural networks to improve simulation of channels affected by water vapour. For RTTOV v14.1 there will be further improvements to simulation accuracy and extension to aerosol simulations.

*Tang modification to Chou-scaling solver*

A recent visiting scientist mission [RD-6] explored the Tang *et al* (2018) modification to the existing Chou-scaling fast IR scattering solver (Chou *et al*, 1999). This is of particular benefit for ice clouds in the far-IR (the focus of the VS mission was in improving the accuracy of scattering simulations for the FORUM mission), but there are suggestions this could benefit scattering simulations at all wavelengths. This will be implemented in v14.0 with the aim of further improving the implementation in a future minor release.

*Emissivity and BRDF atlases*

RTTOV v14.0 supports the CAMEL v3 IR emissivity atlas thus providing users with the latest available land surface emissivity data available. A new feature in v14.0 for the IR emissivity and BRDF atlases is the option to return a nearby emissivity/BRDF value (within a user-specified radius) if the atlas has no data at the given location. This is useful where a first guess emissivity is required in, for example, coastal areas where the atlas land/sea mask may not match that of the NWP model. The implementation is based on code submitted by a user who wanted this capability in RTTOV. The BRDF atlas datasets will be updated for RTTOV v14.1 or v14.2, which has been requested by a number of users.

*PC-RTTOV*

The PC-RTTOV capability will be maintained in RTTOV v14, bringing together support for all previous developments (support for all surface types, variable trace gases, non-local thermodynamic equilibrium effects, aerosol scattering, and cloud scattering) in a single PC coefficient file per sensor. Supported sensors for v14.0 are IASI, IASI-NG, and MTG-IRS. The PC coefficients are trained on updated surface emissivity models and atlases.

*Allocation of memory in RTTOV*

A number of users have reported that the number of memory allocations that occur within RTTOV have a performance impact. RTTOV v14 reduces the number of allocations for certain data structures by allocating a single array with an additional dimension and pointing individual the data structure members to elements of this array. Some users also make use of the ability to allocate the *rttov_traj* “trajectory” structure outside of RTTOV. This contains data structures that hold intermediate calculation results. It can improve performance to allocate it outside of RTTOV and pass it as an argument when making many repeated calls to RTTOV. RTTOV v14 extends this capability to allow the other previously purely internal trajectory data structures (*rttov_traj_dyn*, *rttov_traj_sta*) to be pre-allocated and passed to RTTOV in the same way. This further addresses user concerns regarding memory allocations in RTTOV.

*Replacing HDF5 with netCDF4*

Over the years several users have requested that coefficient files be stored in netCDF format instead of HDF5 as netCDF is commonly installed and can be technically simpler when compiling the code. It is planned to replace the use of HDF5 with netCDF for the core user package: this applies to the various coefficient files and to the emissivity and BRDF atlases. Note that the GUI continues to use HDF5, but this is managed entirely within Python with no Fortran HDF5 dependency. Thus, the only external dependency of the core RTTOV model for users is netCDF.

*CMake*

Two respondents to the 2022 RTTOV user survey [RD-2] specifically asked for CMake to be used for building RTTOV. This will be investigated for a v14 minor release (v14.1 or v14.2). The existing build system will be maintained in parallel, at least initially.

### 3.6 Retirement of deprecated/superseded capabilities

RTTOV has been in development for many years and has been accumulating features, parameterisations, and options over that time, some of which either cannot be maintained due to lack of resources, or which have been superseded or made redundant by newer options, or otherwise have been marked as deprecated in previous releases. It is good practice to remove old/unused/redundant code to reduce the maintenance burden, and to simplify the code where possible. Based on results from the 2022 RTTOV user survey [RD-2], and in the context of the considerations outlined above the following features are planned for removal in RTTOV v14.

*HTFRTC*

There is a problem in the existing implementation of the HTFRTC Principal Components-based model whereby it can return zero radiances for very dry profiles. Resourcing issues have prevented this bug from being resolved, and there are no resources to update HTFRTC in line with the other RTTOV v14 changes described above, so the decision was made to remove HTFRTC from v14. Note that PC-RTTOV remains an option for running PC-based simulations in RTTOV v14.

*Solar single scattering solver*

The single-scattering solver for clouds and aerosols is not accurate and its capabilities are being superseded by the other solvers (DOM, MFASIS-NN). Its removal has been repeatedly advertised to users with no adverse responses.

*MFASIS-LUT fast visible/near-IR cloud solver*

As noted above, the MFASIS-NN neural network-based solver has superseded the look-up table (LUT)-based solver and so MFASIS-LUT has been removed.

*TESSEM2, FASTEM-1/2/3/4 MW sea surface emissivity models*

TESSEM2 has been fully superseded by SURFEM-Ocean. FASTEM has been in RTTOV for many years and has undergone numerous improvements. The earlier versions have been superseded by FASTEM-5/6 and so will be removed.

*JONSWAP solar sea sun glint BRDF option*

The original JONSWAP (Hasselmann *et al,* 1973) solar sea BRDF wave spectrum parameterisation has been superseded by that of Elfouhaily *et al* (1997) and will therefore be removed.

*Removal of options*

RTTOV has a very large number of options (over 60) to configure various aspects of the simulations. It is beneficial to remove options where possible to simplify the interface for users, and so some previously deprecated options have been removed with their default/recommended behaviour implemented:

- *grid_box_avg_cloud* – in v14 users must input grid box average cloud concentrations which is typically what NWP model cloud fields represent.
- *spacetop* – in v13 and earlier, this option was true and there was never a reason for users to set it to false as it would reduce the accuracy of simulations where channel weighting functions were significantly non-zero above the top user level (which is not recommended when running RTTOV anyway).
- *dtau_test* – in v13 this activates or deactivates (v13 default and recommended setting) a check on layer delta-transmittance in the clear-sky integration of the radiative transfer equation. Originally implemented to avoid potential numerical issues, it made the forward model non-differentiable. Assimilation trials have shown no negative impacts of omitting this check, so it has been entirely removed in v14.
- *reg_limit_extrap* – when the top user pressure level lies below the top coefficient pressure level, the code must extrapolate the input profiles at the top of the atmosphere. Originally RTTOV did constant value extrapolation. In v13 this option provided the option to do a more physically realistic extrapolation by following the training profile regression limits. There is no reason to prefer constant value extrapolation to this, so the option has been removed in v14.

## 3.7 RTTOV optical depth coefficient files

For RTTOV v13, a very large variety of optical depth coefficient files are produced. These include files based on the old optical depth predictors (v7, v8, and v9 predictors) and the new v13 predictors. Files can be available supporting different variable gases, and for hyperspectral sensors, on both 54 and 101 coefficient levels. Users often desire continuity in the coefficients they are using operationally meaning requests are received for all types of coefficient files, not only the latest and/or recommended versions. Some users are still using old versions of RTTOV (v12 and earlier) that do not support the v13 predictors. However, it will not be practical to continue supporting the full range of optical depth coefficient files indefinitely, and the wide variety of coefficients is confusing for users.

For RTTOV v14.0, the plan is to produce by default only the recommended coefficients for each sensor as follows:

- **MW sensors**: all 54L, all v13 predictors, all variable $O_3$, all based on top-hat passbands, and additionally files based on measured spectral responses where available (at most two files per sensor).
- **Multi-spectral UV/VIS/IR**: all 54L, all v13 predictors, all variable $O_3$+$CO_2$, additional 7gas files for relevant sensors (at most two files per sensor).
- **Hyperspectral UV/VIS/IR**: all 101L, v13 predictors $O_3$+$CO_2$, v13 and v9 predictors 7gas for relevant sensors (at most three files per sensor).
- **Special cases**: Zeeman, PMR, SSU PMC shift coefficients to remain available with all being updated to v13 predictors as soon as possible.

All other optical depth coefficient files will be deprecated. If/when users request these we will first respond to see if they can move to the recommended files, and if not, only then provide deprecated files. Users will be notified by email and by warnings on the website of the plan to fully retire the deprecated coefficients after the release of RTTOV v15 such that we will no longer generate them.

It is planned during the lifetime of RTTOV v14 to develop new RTTOV v14-only coefficients (i.e., not compatible with v13 and earlier) incorporating various scientific improvements with the aim that these will become the standard for both RTTOV v14 and v15.

## 4. FUNCTIONALITY

RTTOV v14 will perform the following functions:

*Simulation types:*
RTTOV v14 will carry out the following kinds of simulations:

- RQ-4.1 UV, visible and IR (0.23 – 100 microns), and MW (1 – 1000 GHz) clear-sky simulations.
- RQ-4.2 MW clear-sky simulations treating cloud liquid water as an absorber only.
- RQ-4.3 IR simulations with a simple black cloud top at given pressure and with given cloud fraction.
- RQ-4.4 UV/visible simulations with a simple Lambertian cloud top at given pressure and with given cloud fraction.
- RQ-4.5 Scattering simulations at all wavelengths in the presence of aerosols and/or hydrometeors with pre-defined particle optical properties.
- RQ-4.6 Scattering simulations at all wavelengths in the presence of aerosols and/or hydrometeors with user-provided particle optical properties.
- RQ-4.7 Optional treatment of Rayleigh single or multiple scattering for UV and visible simulations.
- RQ-4.8 Optional MW radar simulations in the presence of hydrometeors alongside passive MW scattering simulations.
- RQ-4.9 RTTOV will provide an optional approximate treatment of polarisation in MW scattering simulations.
- RQ-4.10 Principal Component (PC) simulations for hyperspectral IR sounders.

- RQ-4.11 Tangent linear (TL), adjoint (AD) and Jacobian (K) calculations for all simulation types.
- RQ-4.12 Simulation of Zeeman effect in high-peaking SSMI/S, AMSU-A, and ATMS channels.
- RQ-4.13 Simulation of SSU radiances with correction for varying $CO_2$ cell pressure in the instrument.
- RQ-4.14 Optional inclusion of bias correction for non-local thermodynamic equilibrium effects.
- RQ-4.15 Input/output of emissivity, BRDF, and diffuse reflectance for one or more surface types each covering a user-specified fraction of the simulated satellite footprint.
- RQ-4.16 Option to treat the surfaces as Lambertian reflectors, or as partial Lambertian/specular reflectors via a per-surface "specularity" parameter.
- RQ-4.17 Option to specify per-channel effective skin temperatures for each surface instead of a single skin temperature per surface.
- RQ-4.18 Capability to run simulations with multiple threads using OpenMP.
- RQ-4.19 Capability for users to pre-allocate and pass in "trajectory" data structures for single-threaded simulations.
- RQ-4.20 Additional optional outputs: computed geometric heights of pressure levels, diagnosed effective cloud fraction, additional in-atmosphere radiance outputs, data enabling users to carry out dynamic emissivity retrievals.

*Coefficient input/output:*
RQ-4.21 RTTOV v14 will provide subroutines to read RTTOV coefficient and optical property files in ASCII, Fortran unformatted ("binary") and netCDF4 formats. These subroutines will allow a subset of channels to be read from the coefficient files.

RQ-4.22 RTTOV v14 will provide an executable to convert all coefficient and optical property files between ASCII, binary and netCDF4 formats and to optionally extract a subset of channels to a new coefficient file.

*Surface emissivity and reflectance:*
RQ-4.23 RTTOV v14 will provide internal models for sea surface reflectance and emissivity.

RQ-4.24 RTTOV v14 will provide atlases for land surface BRDF and emissivity which can be used to provide BRDF and/or emissivity values for input to RTTOV.

*Ancillary user subroutines and executables:*
RQ-4.25 RTTOV v14 will provide ancillary subroutines and executables to help users make use of the software. These are generally developed in response to requests from users. Key subroutines perform the following tasks: validating input data (profiles, emissivity/reflectance, explicit optical properties) before calling RTTOV, compute satellite zenith and azimuth angles for geostationary sensors, compute solar zenith and azimuth angles, map WMO satellite IDs onto RTTOV (platform, satellite) ID couplets, return emissivities/BRDFs from the RTTOV internal sea surface models without having to run full RTTOV simulations, generate climatological aerosol profiles based on the OPAC components. Key executables perform the following tasks: print out information about a given RTTOV optical depth coefficient file, generate custom aertable (aerosol optical property) files, generate custom hydrotable (hydrometeor optical property) files for microwave sensors.

*RTTOV GUI:*
RQ-4.26 RTTOV v14 will provide a graphical user interface (GUI) which enables direct and Jacobian (K) model simulations to be performed and the results visualised. The RTTOV GUI will support clear-sky and scattering simulations including use of the land surface emissivity and BRDF atlases and will provide a 1DVAR capability.

*RTTOV wrapper:*
RQ-4.27 RTTOV v14 will provide interfaces so that it may be called from C++ and Python. The RTTOV wrapper will support clear-sky and scattering direct and K model simulations, including use of the land surface emissivity and BRDF atlases.

## 5. SOFTWARE ORGANISATION

The Fortran source code is stored in a number of directories under the *src/* directory. The directories group source files broadly according to function. The following directories are included in the package provided to users:

| | |
|---|---|
| *brdf_atlas* | subroutines for accessing the land surface BRDF atlas |
| *coef_io* | subroutines for reading/writing coefficient files |
| *emis_atlas* | subroutines for accessing the land surface emissivity atlases |
| *main* | core subroutines and modules for RTTOV |
| *mw_scatt_coef* | subroutines for generating hydrotable files for microwave sensors |
| *netcdf* | subroutines for input/output in netCDF format |
| *other* | ancillary subroutines which may be helpful for users |
| *parallel* | subroutines defining the parallel (OpenMP) interface to RTTOV |
| *test* | subroutines for testing RTTOV and example code for users |
| *wrapper* | subroutines for the Fortran side of the C++/Python wrapper |

The compilation process creates a library for each subdirectory in *src/*. Users only need to link against those libraries which are used in their application. Information on this will be given in the RTTOV v14 User Guide [RD-7].

In addition to the Fortran source code the package also contains the Python source files for the RTTOV GUI in the top-level *gui/* directory and the C++ and Python source files and example code for the C++/Python wrapper in the top-level *wrapper/* directory.

## 6. INPUTS / OUTPUTS

The primary inputs to RTTOV are the atmospheric and surface variables describing the profile to be simulated. These are grouped into the *rttov_profile* structure which will be described fully in the RTTOV v14 User Guide [RD-7].

The *rttov_direct* (direct model) subroutine accepts as input:

- a structure of type *rttov_options* containing options which configure various aspects of the simulation
- a coefficient structure pre-populated with data for the instrument to be simulated by calling the *rttov_read_coefs* subroutine

- an array of type *rttov_chanprof* containing lists of channels and profiles for every radiance to be simulated, size [*nchanprof*]
- an array of type *rttov_profile* containing the input atmospheric and surface data pertinent to the simulation being performed, size [*nprofiles*]
- an array of type *rttov_emis_refl*, size [*nsurfaces*], containing arrays of input surface emissivities, reflectances, and logical flags indicating whether RTTOV should compute emissivities and reflectances for each channel or if the user is providing the values, each of size [*nchanprof*]
- optional structures containing optical parameters for aerosol and hydrometeor scattering simulations
- optional list of channels for which to calculate reconstructed radiances [*nchannels_rec*]

The outputs are arrays of:
- surface to space transmittances [*nchanprof*]
- level to space transmittances [*nlevels*, *nchanprof*]
- overcast radiances at each input level [*nlayers*, *nchanprof*]
- overcast radiance from user-specified cloud top [*nchanprof*]
- radiances [*nchanprof*]
- brightness temperatures [*nchanprof*] (not for channels below 3 microns)
- bi-directional reflectance factors (BRFs) [*nchanprof*] (solar-affected channels only)
- radar reflectivities and attenuated reflectivities [*nlayers*, *nchanprof*]
- PC scores [*npcscores*, *nprofiles*]
- reconstructed radiances and BTs [*nchannels_rec*, *nprofiles*]
- surface emissivities, BRDFs, and diffuse reflectances (size [*nchanprof*]) used by RTTOV for each surface via the array of type *rttov_emis_refl* [*nsurfaces*]

The tangent linear (TL), adjoint (AD) and Jacobian (K) models accept the same inputs and generate the same outputs as the direct model. They have the following additional inputs and outputs.

The *rttov_tl* (TL model) subroutine additionally accepts as input:
- an array of type *rttov_profile* containing the input atmospheric and surface data perturbations around the input profile, size [*nprofiles*]
- an array of type *rttov_emis_refl*, size [*nsurfaces*], containing arrays of input surface emissivity and reflectance perturbations for those channels where the user provided an input value, each of size [*nchanprof*]

For each of the direct model output arrays listed above, there is a corresponding additional TL output array containing the changes in the output variables of the linearised model corresponding to the input perturbations.

The *rttov_ad* (AD model) subroutine additionally accepts as input:
- input increments either in radiance [*nchanprof*], brightness temperature [*nchanprof*], reflectance (BRF) [*nchanprof*], PC score [*npcscores*, *nprofiles*] or reconstructed radiance [*nchannels_rec*, *nprofiles*] according to the simulation type and user settings. In retrieval/assimilation contexts, the input increments usually corresponding to the gradient of a cost function with respect to the satellite radiances.

The additional AD output arrays are:

- an array of type *rttov_profile* containing the atmospheric and surface variable adjoints (typically the gradient of the cost function with respect to the profile variables), size [*nprofiles*]
- an array of type *rttov_emis_refl,* size [*nsurfaces*], containing arrays of surface emissivity and reflectance adjoints for those channels where the user provided an input value, each of size [*nchanprof*]

The *rttov_k* (Jacobian model) subroutine additionally accepts as input:

- input scale factors (commonly 1) either in radiance [*nchanprof*], brightness temperature [*nchanprof*], reflectance (BRF) [*nchanprof*], PC score [*npcscores*, *nprofiles*] or reconstructed radiance [*nchannels_rec*, *nprofiles*] according to the simulation type and user settings. The values scale the computed Jacobians.

The additional Jacobian output arrays are:

- an array of type *rttov_profile* containing the Jacobians either for radiances [*nchanprof*], brightness temperatures [*nchanprof*], reflectance (BRF) [*nchanprof*], PC scores [*npcscores*, *nprofiles*] or reconstructed radiances [*nchannels_rec*, *nprofiles*] with respect to the atmospheric and surface variables according to the simulation type and user settings.
- an array of type *rttov_emis_refl,* size [*nsurfaces*], containing arrays of surface emissivity and reflectance Jacobians for those channels where the user provided an input value, each of size [*nchanprof*]

# 7. SYSTEM REQUIREMENTS

## 7.1 Language

RQ-7.1 RTTOV is written in Fortran2008 except for the LAPACK routines included in the code (taken from the Fortran77 source). It makes use of commonly supported F95 and F2003 features and a small number of common F2008 intrinsics. The test suite additionally makes use of Perl (v5.6 or later) and Python3. The wrapper supports calls to RTTOV from C++ and Python3, the latter using f2py. The RTTOV GUI is written in Python3 and uses *pyrttov* (the Python interface to RTTOV).

## 7.2 Supported platforms

RQ-7.2 Unix/Linux platforms including Mac OS X and Cray. RTTOV is tested with several compilers listed in the RTTOV v14 User Guide [RD-7]. RTTOV supports parallel processing using OpenMP via RTTOV's parallel interface and is also tested in an operational MPI environment. The full list of platforms/compilers with which RTTOV v14 is successfully tested are given in the Test Log accompanying the RTTOV v14 Test Plan [RD-8].

## 7.3 Performance

RQ-7.3 RTTOV v14 shall be comparable to (or more efficient than) RTTOV v13.2 in speed and memory requirements for equivalent simulations. Comparisons of RTTOV v14.0 and v13.2 in terms of speed and peak memory usage for a variety of simulation types is documented in the Test Log accompanying the RTTOV v14 Test Plan [RD-8].

### 7.4 Interface requirements

RQ-7.4 The interface to RTTOV v14 will necessarily be somewhat different to that of RTTOV v13 due to nature of the changes being implemented. It is intended that the RTTOV v14 interface will be clearer and more consistent than that of v13. A document [RD-9] will be provided in the package comprehensively detailing the technical changes between RTTOV v13 and v14 to aid users in upgrading their code. This will also be of use to v10/v11/v12 users who wish to upgrade directly to v14.

### 7.5 Operational and resource requirements

RQ-7.5 The core RTTOV v14 calculation routines (*rttov_direct/tl/ad/k.F90*) shall be "thread safe" to be able to run on MPP machines.

## 8. DOCUMENTATION

The following user documentation is included in the RTTOV package:

- *NWPSAF_ReleaseNote_RTTOV14.0.pdf* - summary of the package contents and compilation instructions
- *users_guide_rttov14_v1.0.pdf* - user guide giving full details of how to compile and run RTTOV and how to incorporate it into the user's application
- *rttov14_user_interface_changes.pdf* - technical guide help users upgrade from RTTOV v13 (and earlier) to v14
- *rttov-quick-start.pdf* - beginner's guide to help new users get started
- *rttov_gui _v14.pdf* - user guide for RTTOV GUI
- *rttov-wrapper.pdf* - user guide for the C++/Python interface to RTTOV
- *rttov-test.pdf* - detailed description of the RTTOV test suite

## 9. LIST OF REQUIREMENTS

This section details specific requirements to be addressed in the RTTOV v14 Test Plan [RD-8].

RQ-9.1 RTTOV v14 shall perform all the functions listed in Section 4 of this document (requirements RQ-4.1 - RQ-4.27).

RQ-9.2 The software should be successfully built, following the instructions in the RTTOV v14 User Guide [RD-7].

RQ-9.3 The software should meet the system requirements listed in Section 7 of this document (requirements RQ-7.1 - RQ-7.5).

RQ-9.4 The various test suite scripts shall run to completion and shall have no unexpected differences relative to the reference results provided.

RQ-9.5 RTTOV v14 will not be able to replicate radiances from RTTOV v13 as discussed above. The expected differences between RTTOV v13 and v14 will be documented in the RTTOV v14 Science and Validation Report.

## 10. REFERENCES

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