ARTS, the atmospheric radiative transfer simulator, Version 2

Journal of Quantitative Spectroscopy & Radiative Transfer (ISSN: 0022-4073)

Citation for the published paper:
Eriksson, P. ; Buehler, S. ; Davis, C. (2011) "ARTS, the atmospheric radiative transfer simulator, Version 2". Journal of Quantitative Spectroscopy & Radiative Transfer, vol. 112(10), pp. 1551-1558.

http://dx.doi.org/10.1016/j.jqsrt.2011.03.001

ARTS, the Atmospheric Radiative Transfer Simulator, Version 2

P. Eriksson[a,*], S. A. Buehler[b,*], C. P. Davis[c], C. Emde[d], O. Lemke[b]

[a] *Department of Earth and Space Sciences, Chalmers University of Technology, SE-41296 Gothenburg, Sweden*

[b] *Department of Computer Science, Electrical and Space Engineering, Luleå University of Technology, Space Campus 1, SE-98128 Kiruna, Sweden*

[c] *Meteorological Service of New Zealand Ltd., Wellington 6012, New Zealand*

[d] *Meteorological Institute, Ludwig-Maximilians-Universität, Theresienstr. 37, D-80333 Munich, Germany*

Abstract

The second version of the Atmospheric Radiative Transfer Simulator, ARTS, is introduced. This is a general software package for long wavelength radiative transfer simulations, with a focus on passive microwave observations. The core part provides a workspace environment, in line with script languages. New for this version is an agenda mechanism that gives a high degree of modularity. The framework is intended to be as general as possible: the polarisation state can be fully described, the model atmosphere can be one- (1D), two- (2D) or three-dimensional (3D), a full description of geoid and surface is possible, observation geometries from the ground, from satellite, and from aeroplane or balloon are handled, and surface reflection can be treated in simple or complex manners. Remote sensing applications are supported by a comprehensive and efficient treatment of sensor characteristics. Jacobians can be calculated for the most important atmospheric variables in non-scattering conditions. Finally, the most prominent feature is the rigorous treatment of scattering that has been implemented in two modules: A discrete ordinate iterative approach mainly used for 1D atmospheres, and a Monte Carlo approach which is the preferred algorithm for 3D atmospheres. ARTS is freely available, and maintained as an open source project.

---

[*] Corresponding authors

Email addresses: `patrick.eriksson@chalmers.se` (P. Eriksson), `sbuehler@ltu.se` (S. A. Buehler)

Preprint submitted to J. Quant. Spectrosc. Radiat. Transfer *December 13, 2011*

Keywords: atmospheric radiative transfer, emission, polarisation, scattering, sensor modelling, remote sensing
PACS: 42.68.Ay, 42.68.Mj, 42.68.Wt, 92.60.Ta

---

1. Introduction

ARTS is a free open-source software program that simulates atmospheric radiative transfer. It focuses on thermal radiation from the microwave to the infrared spectral range. Version 1.0 of ARTS [1], which handles cases without scattering, was mainly developed between 2000 and 2005. It is well validated [2, 3, 4] and still used, primarily for the analysis of ground-based and satellite-based measurements in the millimetre/submillimetre spectral region [e.g., 5, 6, 7]. A large part of its popularity is due to the retrieval software Qpack [8], which uses ARTS as the forward model. But ARTS version 1.0 has also been used for the simulation of clear-sky broadband energy fluxes in the thermal infrared spectral range [9, 10]. This model version is below denoted as ARTS-1.

From 2002, the ARTS developer community became increasingly interested in the remote sensing of clouds, particularly ice clouds. A main driver was the ESA mission proposal CIWSIR [11], a submillimetre instrument for the characterisation of ice clouds, which required a radiative transfer model that could simulate the scattering by ice particles, including polarisation effects [12, 13].

Another strong driver was the treatment of microwave limb sounders: firstly for the analysis of cloud-affected data from the MLS and Odin-SMR satellite instruments [13, 14, 15, 16]. Secondly, future limb sensors will sample the atmosphere more densely in order to increase the 'tomographic' capability. This and the scattering by clouds demand going beyond a 1D representation of the atmosphere.

The interest in such atmospheric sounding techniques led to an internal fork in the ARTS program development. Active development shifted to version 1.1.x, which included modules to simulate scattering by cloud particles and other significant improvements, while ARTS-1 was maintained to provide a stable version for existing users. The new version with scattering is now complete and stable enough to fully replace the old version. We mark this by calling the latest version ARTS 2.0. The purpose of this article is to present ARTS 2.0, and give an overview of its features, strengths, and limitations. In the remaining text "ARTS" refers to the latest 2.0 version.

2. Overview

2.1. Scope

The ambition is to accommodate simulations of any type of passive longwave observation, and ARTS is designed to have no limitations when it comes to the representation of polarisation state, atmospheric fields and geometrical aspects:

1. The Stokes formalism is used to describe polarisation (Sec. 4.1).
2. The model atmosphere can be represented with a one (1D), two (2D) or three (3D) dimensional view (Sec. 4.2).
3. No assumption of a "flat Earth", the geoid and the surface are either spherical (by definition for 1D), or can be given arbitrary shapes (Sec. 4.2).
4. Radiative transfer calculations can be made from any position and along any direction, as long as the resulting calculations make sense with respect to the model atmosphere (Sec. 4.5).

Individual functions can be limited to some configurations, for example, the Monte Carlo scattering module (Sec. 5.3.2) is restricted to 3D.

As mentioned, handling of scattering is a primary aim of ARTS, where the goal is to allow arbitrary complex scattering properties. This goal has been reached for surface reflection (Sec. 5.4), but not completely for particle scattering (Sec. 4.4). The development has so far focused on exact algorithms and the model's strongest side is that complicated simulations can be performed in a stringent manner. ARTS is thus primarily a research tool. Speed has not been a primary objective, and extremely fast, but approximative, algorithms like RTTOV [17] are not in the scope of ARTS.

The software is mainly developed for remote sensing applications, and an extensive support for inclusion of sensor characteristics is provided (Sec. 5.5). In addition, weighting functions (also called Jacobians) [18, 19] can be obtained for a number of variables in non-scattering conditions.

ARTS comes with a small amount of input data. The purpose of these data is to provide some usage examples, and allow the developers to perform standardised tests before committing changes of the code. Normally, the user has to provide the bulk of input data, such as temperatures, volume mixing ratios and spectroscopic parameters. A noticeable exception is that a number of "absorption models" are built into the model (Sec. 5.1).

2.2. Documentation

The efforts to document ARTS focus on the practical usage of the software. This is mainly achieved through the built-in documentation, that provides a definition and a basic description of individual variables and methods. This documentation can be browsed on-line at `www.sat.ltu.se/arts/docserver`. An introduction to the usage of ARTS on a system level is given by some example cases that are distributed along with the source code.

This article provides a compact overview of ARTS. A more detailed description can be found in the three documents of guide type that are distributed with ARTS. Model definitions and algorithms are described in the 'ARTS user guide' (AUG). The 'ARTS development guide' (ADG) gives practical information for the source code. Background theory for some core subjects is provided by the 'ARTS theory document' (ATD). Some parts are described further, or solely, by dedicated research articles [20, 21, 22, 23]. See further `www.sat.ltu.se/arts/docs/`. Download instructions and technical specifications are found at `www.sat.ltu.se/arts/getarts/`.

2.3. Supporting tools

Functions for creating input files and for reading output files (for e.g. plotting) are provided for two popular higher-level and interactive environments, Python through PyARTS and Matlab through Atmlab. These packages provide also additional features. For example, PyARTS allows the calculation of particle optical properties using the T-matrix code by [24] and a new version of Qpack is being implemented inside Atmlab. The packages can be downloaded from the ARTS home page and are documented separately.

3. The workspace

3.1. ARTS as a scripting language

One of the main goals in the ARTS development was to make the program as flexible as possible, so that it can be used for a wide range of applications and new features can be added in a relatively simple manner. As a result, ARTS behaves like a scripting language. An ARTS controlfile contains a sequence of instructions. When ARTS is executed, the controlfile is parsed, and then the instructions are executed sequentially.

This feature is build around the "workspace" [1]. The basic structure is unchanged from ARTS-1, but some improvements have been introduced.

Regarding the "workspace variables", the set of variables is now not fixed. The user is free to specify new variables, as part of the controlfile operations. User-defined variables can replace any of the pre-defined variables, as long as they are of the same type.

The syntax around the "workspace methods" is also somewhat changed. This change is not described here, it should be clear from the on-line documentation and the example cases (Sec. 2.2).

3.2. Agendas

It became increasingly clear that the workspace methods alone do not provide the flexibility sought. In order to avoid increasingly complex methods, the concept of agendas was introduced. An agenda is a user-defined list of workspace methods, which are executed in sequence to calculate a predefined set of workspace variables from a predefined set of input (workspace) variables. As an example, the absorption is handled by an agenda. Several radiative transfer methods use this agenda as an input variable. When they need local absorption coefficients for a point in the atmosphere, they execute the agenda with the local pressure, temperature, and trace gas volume mixing ratio values as inputs. The agenda then provides absorption coefficients as output. If the absorption is extracted from a pre-calculated lookup table or is calculated from basic spectroscopic data (Sec. 5.1) depends on which methods the user has elected to include in the agenda.

4. Model definitions and input

This section gives some basic model definitions, and comments on mandatory and other input of general character required for a model run. Units used for ARTS specific input and output files, as well as internal definitions of variables, follow the SI system.

4.1. Radiative transfer, nomenclature and variables

ARTS describes (spectral) radiances using the Stokes vector, $\mathbf{I}$. The calculations can be selected to treat one to four elements of the Stokes vector, all methods adjust automatically to this choice. The phrase "scalar radiative transfer" refers to the case when just the first Stokes vector element is considered. The other options are all termed as vector radiative transfer. The four elements of the Stokes vector, $\mathbf{I} = [I, Q, U, V]^T$, are defined as:

$$
\begin{aligned}
I &= I_v + I_h = I_{+45^\circ} + I_{-45^\circ} = I_{lhc} + I_{rhc}, && (1)\\
Q &= I_v - I_h, && (2)\\
U &= I_{+45^\circ} - I_{-45^\circ}, && (3)\\
V &= I_{lhc} - I_{rhc}, && (4)
\end{aligned}
$$

where I_v, I_h, I_{+45°, and I_{-45° are the intensity of the component linearly polarised at the vertical, horizontal, +45° and -45° direction, respectively, and I_{rhc}, and I_{lhc} are the intensity for the right- and left-hand circular components. The definition used here follows [24], see also ATD.

Accordingly, I is the total radiance and the other Stokes elements give the difference between two orthogonal components. Individual components are extracted as combinations of I and the other elements, e.g.

$$I_v = (I + Q)/2. \tag{5}$$

The standard vector radiative transfer equation (VRTE) for cases involving multiple scattering is [24]

$$
\begin{aligned}
\frac{\mathrm{d}\mathbf{I}(\nu, \mathbf{r}, \hat{\mathbf{n}})}{\mathrm{d}s} = \quad & -\mathbf{K}(\nu, \mathbf{r}, \hat{\mathbf{n}})\mathbf{I}(\nu, \mathbf{r}, \hat{\mathbf{n}}) + \mathbf{a}(\nu, \mathbf{r}, \hat{\mathbf{n}})B(\nu, \mathbf{r}) \qquad (6)\\
& + \int_{4\pi} \mathrm{d}\hat{\mathbf{n}}' \mathbf{Z}(\nu, \mathbf{r}, \hat{\mathbf{n}}, \hat{\mathbf{n}}')\mathbf{I}(\nu, \mathbf{r}, \hat{\mathbf{n}}'),
\end{aligned}
$$

where ν is frequency, $\mathbf{r}$ represents the atmospheric position, $\hat{\mathbf{n}}$ is the propagation direction (at $\mathbf{r}$), s is distance along $\hat{\mathbf{n}}$, $\mathbf{K}$ is the extinction matrix, $\mathbf{a}$ is the absorption vector, B is the Planck function and $\mathbf{Z}$ is the phase (or scattering) matrix. This equation assumes local thermodynamic equilibrium and that the scattering events can be treated as incoherent.

Equation 6, or some simplified version of it, is solved, giving simulated radiances. The inclusion of sensor characteristics requires that radiative transfer calculations are performed for a set of monochromatic frequencies, the frequency grid, and a number of pencil beams (Sec. 5.5). The frequency grid is a primary input variable; it determines the frequencies for which absorption and radiative transfer are calculated. The propagation through the atmosphere of the unscattered, but possibly refracted, pencil beam is below denoted as the propagation path.

4.2. Atmospheric and surface variables

Atmospheric quantities can be defined to vary in one, two and three dimensions. The atmospheric dimensionality can thus be 1D, 2D or 3D. Pressure is the vertical coordinate in all cases. The two horizontal dimensions for 3D coincide with standard latitude and longitude. The second dimension for 2D is for simplicity denoted as latitude, but is not demanded to have a direct geophysical interpretation. This latitude can, for example, represent the angular distance inside the plane of a satellite orbit.

Each (active) atmospheric dimension has an associated grid. This gives an atmospheric grid mesh, for which temperature, geometrical altitude (above the geoid) and the volume mixing ratio for the species must be specified. The basic definition of the model atmosphere is completed by the geoid radius and the surface altitude, as a function of latitude and longitude.

The minimum value of the pressure grid sets the upper limit of the model atmosphere (vacuum assumed above). The lower limit for the calculation is set by the ground, which constitutes a surface (with arbitrary topography) at the boundary or inside the atmospheric domain. The atmosphere is undefined outside the latitude and longitude grid ranges.

4.3. Radiative transfer domains

The default assumptions are that scattering can be neglected, and that absorption and emission are unpolarised. More complicated calculation conditions are restricted to a special domain of the atmosphere, introduced initially to handle cloud scattering and consequently called the “cloudbox”. For simplicity, the calculations outside the cloudbox are denoted as “clear sky”.

The vertical limits of the cloudbox are two pressure surfaces. For 1D, the cloudbox extends around the model planet, as implied by the spherical symmetry for this case. For higher atmospheric dimensions, the horizontal limits are found at latitude and longitude grid points. The cloudbox can extend below the surface, or be restricted to the atmosphere. The surface is allowed to cause both scattering and polarisation effects outside the cloudbox.

4.4. Particle optical properties

The optical properties of cloud droplets and ice crystals ($\mathbf{K}$, $\mathbf{a}$ and $\mathbf{Z}$; see Eq. 6) are required as input for scattering calculations. They have to be pre-calculated outside the ARTS program.

For liquid water clouds the droplets are in good approximation of spherical shape and the optical properties can be computed using the well known Mie theory [25]. The Atmlab toolbox includes a Mie program [26] to generate optical properties of spherical particles. Ice crystals have complex hexagonal shapes like solid columns, plates, aggregates etc. The PyARTS package provides tools for the calculation of optical properties of aspherical particles (cylinders, plates, and spheroids) which may be used as approximations for the complex ice crystal shapes. PyARTS uses the T-matrix codes by [24].

ARTS offers the possibility to define an arbitrary number of particle types. For each particle type the user needs to define the particle number density field, so that the desired mixture is obtained. Size and shape are not specified specifically. Instead, each particle type is defined by its single scattering properties. A common assumption is that aspherical cloud particles are randomly oriented, this is one of the options in ARTS. A special feature of ARTS is that it also allows to include oriented, more specifically horizontally aligned, particles. Arbitrarily oriented particles can in principle easily be implemented in ARTS, but it is not done yet for the practical reason that the optical properties for arbitrarily oriented particles require a huge amount of computational memory. See further AUG and [27].

4.5. Observation geometry

There are no intrinsic limitations for the observation geometry. Radiative transfer can be performed for any position inside and above the model atmosphere, and with arbitrary observation direction, as long as the radiative transfer does not reach undefined parts of the atmosphere (Sec. 4.2). As long as this constraint is met, the observation position can be outside the horizontal region covered by the latitude and longitude grids. This option is useful for satellite limb sounding where the distance between the sensor and the practical atmospheric entry point can exceed 1500 km.

The observation geometry is defined by combinations of sensor position and line-of-sight (LOS). The term sensor is used here, but this can be a hypothetical instrument observing monochromatic radiances. Inclusion of sensor characteristics is discussed in Sec. 5.5. The vertical coordinate used for the sensor position is the radius (distance from the origin). Horizontal position is defined by latitude and longitude.

The LOS is specified by a zenith angle, and for 3D also an azimuth angle. The zenith angle is the angle between the observation direction and the radial unit vector. This angle is inside the range [0°,180°]. For 2D, zenith angles down to -180° are also defined, where a positive / negative value signifies an observation direction towards higher / lower latitudes. The azimuth angle is defined as the clockwise angle between the observation direction and meridional plane north of the observation point. Westward observations have negative azimuth angles and the allowed range is [-180°,180°].

ARTS is designed to handle a complete measurement sequence by default, and the involved variables can hold a series of position and LOS combinations. Each combination of position and LOS is denoted as a measurement block. This reflects that the operations for a single position and LOS combination can involve numerous radiance calculations, and that the output can correspond to several measurement spectra. A static sensor is assumed inside each measurement block and any shift of the observation position requires a new such block. See further Sec. 5.5.

5. Calculation algorithms

5.1. Gas absorption

The actual gas absorption calculation routines in ARTS are identical to those in ARTS-1 [1]. In particular, ARTS can do line-by-line absorption calculations, but includes also some predefined complete absorption models and continua. The absorption can be calculated explicitly for each position along the propagation path, that gives highest possible accuracy but slow calculations. As a more rapid alternative, a lookup table approach has been implemented, which stores pre-calculated absorption cross-sections as a function of pressure, temperature, and water vapour concentration [28].

5.2. Ray tracing

The radiative transfer equation is solved along a pre-calculated propagation path. Such a path is basically described by a set of positions and the distance between these points. The ray inside each grid box is calculated separately. There are two reasons for this. Firstly, the DOIT algorithm (Sec. 5.3.2) operates only with such local propagation paths. Secondly, interpolation tends to cause a smoothing of atmospheric structures and to decrease this effect it is desirable that the propagation points include all crossings with the atmospheric grids. A step-wise approach is then required, considering that these points can not be calculated in an analytical manner with refraction. The same applies for the crossings with pressure surfaces, even without refraction, as ARTS allows the radius for each surface to vary.

The details of the path calculations are described in AUG, and are not repeated here. Refraction is so far only handled in a very straightforward, but inefficient, way, and further work is needed on this point.

5.3. Radiative transfer algorithms

5.3.1. Clear-sky

As described in Sec. 4.3, the term “clear sky” refers in ARTS to the domain outside the cloudbox. For this domain it is assumed that scattering can be neglected and that absorption (and thus also emission) is unpolarised. However, the radiative transfer must be performed in a vector manner, to correctly propagate polarisation effects generated inside the cloudbox and by the surface.

This part is totally reimplemented but the calculations are basically performed as in ARTS-1, including the calculation of weighting functions [1]. As emission is unpolarised for this domain, only transmission has to be considered for the Q, U and V elements of the Stokes vector (i.e. the Beer-Lambert law). An analytical approach can be used for the weighting functions of some variables, so far implemented in ARTS for gas concentrations and atmospheric temperatures (neglecting non-local effects due to refraction and hydrostatic equilibrium).

5.3.2. Cloud scattering

The most unique feature of ARTS is the possibility to handle scattering in a rigorous manner. In fact, two algorithms that solve the VRTE (Eq. 6) have been implemented as part of the development of ARTS. One of the algorithms is based on a Discrete Ordinate ITerative (DOIT) scheme [20]. The second algorithm applies Monte Carlo (MC) integration with importance sampling [21]. The DOIT scheme calculates the entire radiation field within the ‘cloudbox’ and is the preferred method for 1-D calculations. The MC scheme calculates the Stokes’ Vector for only a single viewing direction, but, due to the efficiency of Monte Carlo methods for highly dimensioned integration, is the preferred method for 3-D calculations. The MC algorithm is not confined to the cloudbox, and handles surface effects in a similar fashion to cloud scattering and emission. Also, if desired, scalar antenna response functions can be handled by Monte Carlo integration over viewing directions.

DOIT and MC make use of the general features of ARTS described in this article, and we refer to [20, 21], AUG and ATD for details of the specific algorithms. Both DOIT and MC have been applied for theoretical studies, as well as practical retrievals, for example [29, 30, 11, 31, 15, 32] and [14, 33, 13, 34, 16], respectively.

5.4. Surface scattering

The Stokes vector for upwelling radiation from the surface, $\mathbf{I}^u$, in the direction of $\hat{\mathbf{n}}$, is calculated as

$$\begin{aligned} \mathbf{I}^u(\nu, \hat{\mathbf{n}}) &= \mathbf{I}^e(\nu, \hat{\mathbf{n}}) + \int_{2\pi} \mathrm{d}\hat{\mathbf{n}}' \mathbf{R}(\nu, \hat{\mathbf{n}}, \hat{\mathbf{n}}') \mathbf{I}^d(\nu, \hat{\mathbf{n}}') \\ &\approx \mathbf{I}^e(\nu, \hat{\mathbf{n}}) + \sum_{i=1}^{n} \mathbf{R}_i(\nu, \hat{\mathbf{n}}, \hat{\mathbf{n}}') \mathbf{I}_i^d(\nu, \hat{\mathbf{n}}') \end{aligned} \tag{7}$$

The first term, $\mathbf{I}^e$, is surface emission for the direction of concern. The second term treats the reflection of down-welling radiation, where we use a discrete approximation. This equation can be compared to the last term of Eq. 6, that describes scattering into the line-of-sight. The main differences are that this integration is performed only over a half sphere and $\mathbf{R}$ is denoted as the bidirectional polarised reflectance distribution function (BPDF).

Accordingly, the down-welling radiation, $\mathbf{I}^d$, is calculated for n directions, giving $\mathbf{I}_i^d$. The set of $\mathbf{I}_i^d$ are weighted with the matrices $\mathbf{R}_i$ that are a combination of the BPDF and the solid beam angle that each direction i represents.

The down-welling term of Eq. 7 vanishes if the surface is treated to be a blackbody. For surfaces that can be treated as lacking roughness, n is one and $\hat{\mathbf{n}}'$ is the specular direction. The required value for n and the best selection of the $\hat{\mathbf{n}}'$-directions for other situations is open for experimentation. Methods for blackbody, specular and Lambertian surface conditions have been implemented (applied equations found in AUG).

As noted in Sec. 5.3.2, the MC algorithm has its own way of handling surface scattering: using Monte Carlo integration to evaluate the integral in Eq. 7.

5.5. Sensor characteristics

Several instrumental effects can be expressed as

$$\int r(x) I(x) \, \mathrm{d}x, \tag{8}$$

where r is the instrument's response function, I is the radiance and x is frequency or some other variable, depending on which response that is treated.

The normal case is that simulations are repeated for the same sensor characteristics, and a direct implementation of Eq. 8 is normally not most efficient. In practise, I is a discrete quantity, and we have a set of values; I_i. The approach taken in ARTS is based on the observation that the practical calculation of Eq. 8 can be written as

$$\sum_i h_i I_i. \tag{9}$$

This expression assumes that r is independent of I, which is generally valid. The summation weights h_i are pre-calculated and stored in a matrix $\mathbf{H}$. The $\mathbf{H}$ of each sensor component can be calculated separately:

$$\mathbf{H} = \mathbf{H}_n \ldots \mathbf{H}_2 \mathbf{H}_1, \tag{10}$$

where n is the number of sensor components considered. The inclusion of sensor characteristics is then simply made as

$$\mathbf{y} = \mathbf{H}\mathbf{i}, \tag{11}$$

where $\mathbf{i}$ is a vector, where the Stokes vectors from each monochromatic radiance calculation are appended, and $\mathbf{y}$ is the final "measurement vector". This approach was introduced by [35] and elaborated further in [22].

The method presented in [23] to efficiently handle broadband infrared channels is also implemented in ARTS. The approach can be seen as an extension of Eq. 11, where the frequencies of $\mathbf{i}$ and the "weights" in $\mathbf{H}$ are selected in parallel. This in order to approximate Eq. 8 over a large range of atmospheric conditions with the lowest possible number of monochromatic frequencies (length of $\mathbf{i}$).

5.6. Transmission and batch calculations

The standard ARTS case is measurements of direct or scattered emission, but also pure transmission calculations can be treated. For example, it possible to simulate solar occultation and satellite-to-satellite transmissions. This includes particle effects, as long as the (re-)scattering into the line-of-sight can be neglected.

ARTS includes now a very general mechanism for batch calculations. This is handled by an agenda (Sec. 3.2) that contains the methods that should be executed for each batch case. Batch calculations are particularly efficient with absorption lookup tables (Sec. 5.1), since the table has to be calculated (or read from file) only once, and can then be used for all cases. A typical application of this is to simulate satellite measurements for a large number of atmospheric scenarios.

5.7. Radiance units

The flexibility of ARTS has the consequence that there is no fixed unit for the measurement vector $\mathbf{y}$. The unit depends primarily on the method selected to set the emission source term, but the sensor response matrix ($\mathbf{H}$) can also include operations that change the unit.

The standard definition inside ARTS of the Planck function is

$$B(T) = \frac{2h\nu^3}{c^2(exp(h\nu/k_BT) - 1)}, \tag{12}$$

where h is the Planck constant, c the speed of light and k_B the Boltzmann constant. This expression gives the (total) power per unit frequency per unit area per solid angle and the resulting unit is $\mathrm{W/(m^2\,Hz\,sr)}$. As long as Eq. 12 is followed, ARTS supports conversion to the following units:

$\mathbf{W/(m^2\,m\,sr)}$, power per unit wavelength per unit area per solid angle
$\mathbf{W/(m^2\,m^{-1}\,sr)}$, as above but per unit wavenumber
RJBT, brightness temperature (T_B) following the Rayleigh-Jeans approximation of the Planck function [K]
PlanckBT, brightness temperature following the Planck function [K]

The two first conversions correspond to linear mappings, and a common rescaling factor can be applied for all Stokes elements, polarisation components and the Jacobian. The conversion to brightness temperatures is more complex. In the text below, all primed quantities (I', Q', I'_v, ...) refer to brightness temperatures (RJ or Planck), whereas all unprimed quantities (I, Q, I_v, ...) refer to radiances.

5.7.1. Stokes element I

The first Stokes element is converted to PlanckBT by inverting Eq. 12,

$$I' = B^{-1}(I) = \frac{h\nu}{k_B \ln((p_n h\nu^3/c^2 I) + 1)}, \tag{13}$$

while the conversion to RJBT uses the standard approximative expression

$$I' = \frac{c^2}{p_n \nu^2 k_B} I. \tag{14}$$

The factor p_n, representing the number of polarisation modes [36], is introduced for reasons of generality (see below). For I, $p_n = 2$ in both equations above (to match Eq. 12).

The conversion of the Jacobian to PlanckBT requires further considerations. The derivative of a radiance in PlanckBT, with respect to a variable x, can be formulated as

$$\frac{\partial I'}{\partial x} = \frac{\partial B^{-1}(I)}{\partial x} = \frac{\partial B^{-1}(I)}{\partial I}\frac{\partial I}{\partial x}. \tag{15}$$

The term $\partial I/\partial x$ is the weighting function for the original unit, that shall be converted to PlanckBT. The conversion term can be derived to be

$$\frac{\partial B^{-1}}{\partial I} = \frac{k_B\left[B^{-1}(I)\right]^2}{h\nu I(1 + (c^2 I/2h\nu^3))}. \tag{16}$$

5.7.2. Stokes elements Q, U and V

The conversion of Q, U and V to RJBT is made exactly as for I. That is, Eq. 14 is applied with $p_n = 2$. This deviates from e.g. [36] (setting $p_n = 1$ for these Stokes elements), but is preferred for reasons of generality. A practical consideration for the Stokes vector is that the ratio between the elements must be the same independent of the selected unit. Otherwise it would be needed to adapt optical properties, e.g. $\mathbf{K}$ (Eq. 6), to the selected unit. Another way to express this is that, in the Rayleigh-Jeans limit, the same result shall be obtained if Eq. 12 is used and radiances are converted to RJBT, as if the emission source term (B) is replaced by the physical temperature (T). ARTS allows the latter, see [37] for a discussion of this choice. (It should be noted that these two options do not generally give the same T_B).

As Eq. 13 is a non-linear mapping, it can not be applied directly on Q, U and V. To maintain the basic properties of the Stokes vector, Q is converted to PlanckBT as (cf. Eqs. 2 and 5)

$$Q' = B^{-1}\left(\left[I + Q\right]/2\right) - B^{-1}\left(\left[I - Q\right]/2\right). \tag{17}$$

The conversion of weighting functions must be done in a similar manner

$$\frac{\partial Q'}{\partial x} = \left[\left.\frac{\partial B^{-1}}{\partial I}\right|_{(I+Q)/2} + \left.\frac{\partial B^{-1}}{\partial I}\right|_{(I-Q)/2}\right]\frac{\partial Q}{\partial x}. \tag{18}$$

The elements U and V are treated likewise.

5.7.3. Individual polarisation components

The measurement vector **y** can contain either Stokes elements (I, Q, ...) or individual polarisation components (I_v, I_h, ..., see Sec. 4.1). In the later case this is taken as a calibrated observation and, as the data correspond to a single polarisation mode, the conversion to T_B must be adapted. The reference for the conversion is then the blackbody radiation for a single polarisation mode, that is a factor 2 smaller than Eq. 12. The conversion from radiance to T_B is thus made through Eqs. 13 and 14 with $p_n = 1$.

If individual polarisation components are extracted outside ARTS, it is important to note that the definitions above have the consequence that Eq. 5 can not be applied if the data have been converted to T_B. As example, the brightness temperature for the vertical linear component is obtained as

$$I'_v = I' + Q', \tag{19}$$

which differs from Eq. 5 with a factor of two.

6. Conclusions

The first version of ARTS (ARTS-1) was a traditional microwave to infrared clear-sky forward model; it was 1D and had no treatment of scattering. The main novelty of ARTS-1 was the introduction of the workspace. However, the ambition of easily extendable software was not fully met by ARTS-1, and the concept was for this version extended by an agenda mechanism. Our experience so far is that the desired degree of modularity has been reached.

The new ARTS version (2.0) is a state-of-the-art radiative transfer model for the thermal spectral region, as it combines the following features:

- The model atmosphere can be 1D, 2D or 3D. Tomographic limb sounding retrievals require 2D or 3D, and rigorous cloud scattering simulations are only possible in 3D.

- Spherical geoid and surface are throughout default. For 2D and 3D more complex topography are also possible. A ‘flat Earth’ is not a viable option for limb sounding.

- Radiative transfer can be made for 1 to 4 Stokes elements. Polarisation effects can thus be fully described.

- Basically no restriction in complexity of surface reflection (but is currently handled only in a simplistic manner).

- For particle single scattering properties, not only the standard assumption of spherical or completely randomly oriented particles, but also the case of horizontally aligned particles is handled.

- Two modules for solving radiative transfer with particle scattering: MC and DOIT. Both modules lack intrinsic approximations, and have been verified by practical retrievals [15, 16].

- Sensor responses can be incorporated in an efficient manner [22, 23].

Another way to judge the scientific merits of ARTS-2.0 is the fact that it has already been used for a number of scientific publications. Direct usage of ARTS-2.0 includes [38, 14, 29, 39, 33, 11, 13, 40, 15, 30, 31, 34, 32, 41, 42, 43, 16, 44], and indirect usage is found in yet more journal articles.

The main limitations of ARTS-2.0 are:

- Physical mechanisms not yet implemented include non-local thermodynamic equilibrium and polarised gas absorption.

- Particle single scattering properties must be calculated externally.

- Extremely fast calculations are not within the present scope of ARTS. The same applies to calculation of radiative fluxes and cooling rates.

- Weighting functions can be obtained, but so far only for a limited number of variables under non-scattering conditions.

The web address for ARTS is `www.sat.ltu.se/arts`, where the software can be downloaded freely and additional documentation is found. Please, note the "code of conduct" found on the web site, asking users to cite this and the relevant module specific articles [at the time of writing: 20, 21, 22, 23, 28].

Acknowledgements

First of all, we thank all others that have contributed to the ARTS development over the years, particularly Hermann Berg, Mattias Ekström, Axel von Engeln, Wolfram Haas, Carlos Jiménez, Viju John, Nikolay Koulev, Thomas Kuhn, Mashrab Kuvatov, Christian Melsheimer, Mathias Milz, Randall Skelton, Claas Teichmann, and Sreerekha T.R. The second acknowledgement is due to all those in the ARTS user community that have contributed interesting use cases, applications, and discussions on the ARTS mailing list (`arts-users@www.sat.ltu.se`). Seeing the model being used is the biggest reward for us who have developed it!

Last but not least, we acknowledge our funding agencies. The ESA study 'Development of a Radiative Transfer Model for Frequencies between 200 and 1000 GHz' (contract 17632/03/NL/FF) was especially valuable. Further, direct or indirect support has been provided by the Swedish National Space Board (e.g. 59/07 and 92/08) and by the Swedish Research Council (2007-3720 and 2007-5370), through different contracts at both the Swedish groups. Development of the ARTS-MC algorithm was largely funded by the UK Natural Environment Research Council.

References

[1] S. A. Buehler, P. Eriksson, T. Kuhn, A. von Engeln, and C. Verdes. ARTS, the Atmospheric Radiative Transfer Simulator. *J. Quant. Spectrosc. Radiat. Transfer*, 91:65–93, 2005.

[2] C. Melsheimer, C. Verdes, S. A. Buehler, C. Emde, P. Eriksson, D. G. Feist, S. Ichizawa, V. O. John, Y. Kasai, G. Kopp, N. Koulev, T. Kuhn, O. Lemke, S. Ochiai, F. Schreier, T. R. Sreerekha, M. Suzuki, C. Takahashi, S. Tsujimaru, and J. Urban. Intercomparison of general purpose clear sky atmospheric radiative transfer models for the millimeter/submillimeter spectral range. *Radio Sci.*, 40:RS1007, 2005.

[3] S. A. Buehler, N. Courcoux, and V. O. John. Radiative transfer calculations for a passive microwave satellite sensor: Comparing a fast model and a line-by-line model. *J. Geophys. Res.*, 111, 2006.

[4] R. Saunders, P. Rayer, P. Brunel, A. von Engeln, N. Bormann, L. Strow, S. Hannon, S. Heilliette, Xu Liu, F. Miskolczi, Y. Han, G. Masiello, J.-L. Moncet, G. Uymin, V. Sherlock, and D. S. Turner. A comparison of radiative transfer models for simulating Atmospheric Infrared Sounder (AIRS) radiances. *J. Geophys. Res.*, 112, 2007.

[5] J. Urban, N. Lautié, E. Le Flochmoën, C. Jiménez, P. Eriksson, E. Dupuy, L. El Amraoui, M. Ekström, U. Frisk, D. Murtagh, J. de La

Noë, M. Olberg, and P. Ricaud. Odin/SMR limb observations of stratospheric trace gases: Level 2 processing of ClO, N_2O, O_3, and HNO_3. *J. Geophys. Res.*, 110:D14307, July 2005.

[6] V. O. John and S. A. Buehler. Comparison of microwave satellite humidity data and radiosonde profiles: A survey of European stations. *Atmos. Chem. Phys.*, 5:1843–1853, 2005. SRef-ID:1680-7324/acp/2005-5-1843.

[7] V. O. John and S. A. Buehler. The impact of ozone lines on AMSU-B radiances. *Geophys. Res. Lett.*, 31, 2004.

[8] P. Eriksson, C. Jiménez, and S. A. Buehler. Qpack, a tool for instrument simulation and retrieval work. *J. Quant. Spectrosc. Radiat. Transfer*, 91:47–64, 2005.

[9] S. A. Buehler, A. von Engeln, E. Brocard, V. O. John, T. Kuhn, and P. Eriksson. Recent developments in the line-by-line modeling of outgoing longwave radiation. *J. Quant. Spectrosc. Radiat. Transfer*, 98(3):446–457, 2006.

[10] V. O. John, S. A. Buehler, A. von Engeln, P. Eriksson, T. Kuhn, E. Brocard, and G. Koenig-Langlo. Understanding the variability of clear-sky outgoing long-wave radiation based on ship-based temperature and water vapor measurements. *Q. J. R. Meteorol. Soc.*, 132(621):2675–2691, 2006.

[11] S. A. Buehler, C. Jimenez, K. F. Evans, P. Eriksson, B. Rydberg, A. J. Heymsfield, C. Stubenrauch, U. Lohmann, C. Emde, V. O. John, T. R. Sreerekha, and C. P. Davis. A concept for a satellite mission to measure cloud ice water path and ice particle size. *Q. J. R. Meteorol. Soc.*, 133(S2):109–128, 2007.

[12] J. Miao, K.-P. Johnsen, S. A. Buehler, and A. Kokhanovsky. The potential of polarization measurements from space at mm and sub-mm wavelengths for determining cirrus cloud parameters. *Atmos. Chem. Phys.*, 3:39–48, 2003.

[13] C. P. Davis, K. F. Evans, S. A. Buehler, D. L. Wu, and H. C. Pumphrey. 3-D polarised simulations of space-borne passive mm/sub-mm midlatitude cirrus observations: A case study. *Atmos. Chem. Phys.*, 7:4149–4158, 2007.

[14] C. P. Davis, D. L. Wu, C. Emde, J. H. Jiang, R. E. Cofield, and R. S. Harwood. Cirrus induced polarization in 122 GHz Aura Microwave Limb Sounder radiances. *Geophys. Res. Lett.*, 32, 2005.

[15] P. Eriksson, M. Ekström, B. Rydberg, and D. P. Murtagh. First Odin sub-mm retrievals in the tropical upper troposphere: Ice cloud properties. *Atmos. Chem. Phys.*, 7(2):471–483, 2007.

[16] B. Rydberg, P. Eriksson, S. A. Buehler, and D. P. Murtagh. Non-gaussian bayesian retrieval of tropical upper tropospheric cloud ice and water vapour from Odin-SMR measurements. *Atmos. Meas. Tech.*, 2(2):621–637, 2009.

[17] R. Saunders, M. Matricardi, and P. Brunel. An improved fast radiative transfer model for assimilation of satellite radiance observations. *Q. J. R. Meteorol. Soc.*, 125:1407–1425, 1999.

[18] C. D. Rodgers. Characterization and error analysis of profiles retrieved from remote sounding measurements. *J. Geophys. Res.*, 95(D5):5587–5595, 1990.

[19] C. D. Rodgers. *Inverse methods for atmospheric sounding: Theory and practise.* World Scientific Publishing Co. Pte. Ltd: Singapore, 2000.

[20] C. Emde, S. A. Buehler, C. Davis, P. Eriksson, T. R. Sreerekha, and C. Teichmann. A polarized discrete ordinate scattering model for simulations of limb and nadir longwave measurements in 1D/3D spherical atmospheres. *J. Geophys. Res.*, 109(D24):D24207, 2004.

[21] C. Davis, C. Emde, and R. Harwood. A 3D polarized reversed Monte Carlo radiative transfer model for mm and sub-mm passive remote sensing in cloudy atmospheres. *IEEE Trans. Geosci. Remote Sensing*, 43(6):1096–1101, May 2005.

[22] P. Eriksson, M. Ekström, S. A. Buehler, and C. Melsheimer. Efficient forward modelling by matrix representation of sensor responses. *Int. J. Remote Sensing*, 27(9–10):1793–1808, 2006.

[23] S. A. Buehler, V. O. John, A. Kottayil, M. Milz, and P. Eriksson. Efficient radiative transfer simulations for a broadband infrared radiometer - Combining a weighted mean of representative frequencies approach

with frequency selection by simulated annealing. *J. Quant. Spectrosc. Radiat. Transfer*, 111:602–615, 2010.

[24] M. I. Mishchenko, L.D. Travis, and A.A. Lacis. *Scattering, absorption, and emission of light by small particles*. Cambridge University Press, 2002.

[25] G. Mie. Beiträge zur Optik trüber Medien, speziell kolloidaler Metallösungen. *Ann. Phys.*, 330:377–445, 1908.

[26] C. Mätzler. *MATLAB functions for Mie scattering and absorption*. University of Bern, version 2 edition, 2002.

[27] A. Battaglia, C. Simmer, S. Crewell, H. Czekala, C. Emde, F. Marzano, M. Mishchenko, J. Pardo, and C. Prigent. Emission and scattering by clouds and precipitation. In C. Mätzler, editor, *Thermal microwave radiation: Applications for remote sensing*, pages 101–233. The Institution of Engineering and Technolog, London, UK, 2006.

[28] S. A. Buehler and P. Eriksson. Absorption lookup tables in the radiative transfer model ARTS. *J. Quant. Spectrosc. Radiat. Transfer*, submitted, 2010.

[29] M. Hoepfner and C. Emde. Comparison of single and multiple scattering approaches for the simulation of limb-emission observations in the mid-IR. *J. Quant. Spectrosc. Radiat. Transfer*, 91(3):275–285, March 2005.

[30] L. Pietranera, S. A. Buehler, P. G. Calisse, C. Emde, D. Hayton, V. O. John, B. Maffei, L. Piccirillo, G. Pisano, G. Savini, and T. R. Sreerekha. Observing CMB polarisation through ice. *Mon. Not. R. Astron. Soc.*, 376:645–650, 2007.

[31] B. Rydberg, P. Eriksson, and S. A. Buehler. Prediction of cloud ice signatures in sub-mm emission spectra by means of ground-based radar and in-situ microphysical data. *Q. J. R. Meteorol. Soc.*, 133(S2):151–162, 2007.

[32] T. R. Sreerekha, S. A. Buehler, U. O'Keeffe, A. Doherty, C. Emde, and V. O. John. A strong ice cloud event as seen by a microwave satellite sensor: Simulations and observations. *J. Quant. Spectrosc. Radiat. Transfer*, 109(9):1705–1718, 2008.

[33] A. Battaglia, C. P. Davis, C. Emde, and C. Simmer. Microwave radiative transfer intercomparison study for 3-D dichroic media. *J. Quant. Spectrosc. Radiat. Transfer*, 105(1):55–67, 2007.

[34] I. S. Adams, P. Gaiser, and W. L. Jones. Simulation of the Stokes vector in inhomogeneous precipitation. *Radio Sci.*, 43(5), 2008.

[35] P. Eriksson, F. Merino, D. Murtagh, P. Baron, P. Ricaud, and J. de La Noë. Studies for the Odin sub-millimetre radiometer: 1. Radiative transfer and instrument simulation. *Can. J. Phys.*, 80:321–340, 2002.

[36] C. Mätzler and C. Melsheimer. Radiative transfer and microwave radiometry. In C. Mätzler, editor, *Thermal microwave radiation: Applications for remote sensing*, pages 1–23. The Institution of Engineering and Technolog, London, UK, 2006.

[37] Q. Liu, F. Weng, and Y. Han. Note: Conversion issues between microwave radiance and brightness temperature. *J. Quant. Spectrosc. Radiat. Transfer*, 109:1943–1950, 2008.

[38] C. Emde, S. A. Buehler, P. Eriksson, and T. R. Sreerekha. The effect of cirrus clouds on limb radiances. *J. Atmos. Res.*, 72:383–401, 2004.

[39] C. Teichmann, S. A. Buehler, and C. Emde. Understanding the polarization signal of spherical particles for microwave limb radiances. *J. Quant. Spectrosc. Radiat. Transfer*, 101(1):179–190, September 2006.

[40] M. Ekström, P. Eriksson, B. Rydberg, and D. P. Murtagh. First Odin sub-mm retrievals in the tropical upper troposphere: Humidity and cloud ice signals. *Atmos. Chem. Phys.*, 7(2):459–469, 2007.

[41] A. Haefele, E. De Waehter, K. Hocke, N. Kmpfer, G.E. Nedoluha, R.M. Gomez, R. Eriksson, R. Forkman, A. Lambert, and M.J. Schwartz. Validation of ground-based microwave radiometers at 22 GHz for stratospheric and mesospheric water vapor. *J. Geophys. Res.*, 114(23), 2009.

[42] R. C. Harlow. Millimeter microwave emissivities and effective temperatures of snow-covered surfaces: Evidence for Lambertian surface scattering. *IEEE Trans. Geosci. Remote Sensing*, 47:1957–1970, 2009.

[43] M. Milz, S. A. Buehler, and V. O. John. Comparison of AIRS and AMSU-B monthly mean estimates of upper tropopsheric humidity. *Geophys. Res. Lett.*, 2009.

[44] G. Holl, S. A. Buehler, B. Rydberg, and C. Jiménez. Collocating satellite-based radar and radiometer measurements - methodology and usage examples. *Atmos. Meas. Tech.*, 3(3):693–708, 2010.