ABSTRACT:
A toolbox for microwave radiative transfer through planetary atmospheres has been developed. The toolbox consists of the propagation model, ARTS, including a number of test and demo cases and a collection of data to run the model. The propagation model has been largely extended during the course of the project. Added or largely revised major features are (a) handling (general) planetary atmospheres (including methods for line absorption, continuum, and refractivity calculations in non-standard air mixtures; revised spectroscopic line catalogue format; planetary “constants” like size/shape, gravitational constant, etc. as input parameters), (b) modelling of radio link budgets (calculation of transmitter-receiver paths, algorithms to determine free space loss, defocusing loss, extra path delay, bending angles), (c) modelling wind and other Doppler effects, Faraday rotation, improved methods for calculations including clouds/aerosols, and extended output parameter capabilities including output of parameters decomposed along the path. Demos cases, specifically developed for the toolbox, are an integrated part of the propagation model. Passive clearsky observation setups and radio occultation cases for the different planets, a case demonstrating usage of 3D data and wind-affected radiative transfer in a 3D space as well as a link budget case in 3D space are available. The data package includes spectroscopic data (line catalogue and collision induced absorption continuum data) and atmospheric scenarios for the considered planets Earth, Venus, Mars, Jupiter (including temperature, volume mixing ratio, wind, electron density, magnetic field, and cloud/haze/dust data as well as some selected surface property information). Validation of the toolbox has been performed in the form of verification of certain features of the propagation model (particular such that have been newly implemented for the toolbox), sensitivity studies (particularly regarding the atmospheric state data provided with the toolbox) and comparisons to simulations from other propagation models and to observations.

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Executive Summary (D13b)

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1 Project Objectives

Various advanced electromagnetic propagation models adapted to Earth or to various planetary atmospheres do exist. Often, these models are designed for a narrow band of the electromagnetic spectrum, a specific atmosphere, or a specific measurement system, i.e., for a narrow range of applications. Other models are dedicated to be used with sophisticated inversion algorithms for accurate retrievals of atmospheric parameters. Demanding high accuracy makes them bulky and slow. For preliminary investigations on the potential of innovative remote sensing techniques and sensitivity analyses, tools that allow a quick estimation of the main microwave propagation parameters and are applicable for a wide range of conditions are desirable.

The objective of this study has been to design and build up a fast and easy-to-use propagation model available to ESA as an in-house tool supporting the definition of future missions for Earth observation as well as remote sensing of solar system planets. The model shall be applicable for propagation calculations of microwave to sub-millimetre electromagnetic radiation in the atmospheres of the planets Earth, Mars, Venus, and Jupiter. It shall cover a wide range of applications, i.e., allow to calculate basic radiative quantities (e.g., total and path segment decomposed attenuation) as well as to simulate measurements by passive instruments and of radio link properties. According to the Statement of Work (SoW) issued by ESA, demanded functionality includes polarimetry, modelling of absorption/emission as well as scattering, multi-dimensionality, ray tracing for single- and both-side edged paths, wind Doppler effects. Furthermore, data to run the propagation model from (e.g., fields of atmospheric temperature, gaseous constituents and clouds/dust, wind, electron density) shall be included in the toolbox.

2 Approach

The Atmospheric Radiative Transfer Simulator (ARTS) (Buehler et al., 2005; Eriksson et al., 2011) was recognised as a reference document by the Statement of Work. The ARTS model in its pre-project state (Sec. 3.1), already comprised many of the functionalities requested by the SoW, hence formed an excellent base for the project. The intention was to build on this comprehensive model, and to extend and improve the it. A number of adaptations and extensions of the ARTS model were identified to be necessary to meet the toolbox requirements.

This primarily regarded the replacement of algorithms and data contain-
ing implicit assumptions on the planet’s atmospheric conditions, e.g., the composition of “air” (Sec. 3.2). Active signals had not yet been in the scope of ARTS before this project. However, it was considered that modelling of active techniques could make use of existing ARTS functionality, e.g., the calculation of attenuation along a propagation path. Sec. 3.3 summarises the new capabilities in active signal modelling. An overview of further significant extensions is presented in Sec. 3.4.

Additional data as input to the model had to be collected, which regarded data for describing the non-Earth planets, e.g., atmospheric scenarios, as well as spectroscopic data applicable for general planetary conditions (Sec. 3.5).

The consortium for the project was built around ARTS development team members (J. Mendrok, S. Buehler of LTU, Sweden; P. Eriksson of CUT, Sweden). External experts were consulted and involved with focus on compilation of spectroscopic data (A. Perrin of LISA, France) and planetary scenarios (P. Hartogh, L. Rezac of MPS, Germany).

3 Toolbox development

3.1 Pre-project status of ARTS

ARTS is a radiative transfer (RT) model for the microwave to thermal infrared spectral range. The basic principle of ARTS is to provide a code applicable for many different applications. For this reason string emphasis is placed on modularity, extendability, and generality.

Generality includes that — if and as far as practically possible — ARTS is based on physical principles rather than on empirical relations. From the user point of view, modularity is reflected in the scripting language style of the user interface. That is, there is no fixed path through the program for an ARTS run, but the ARTS controlfile contains a sequence of instructions to be executed. This provides a large flexibility in the type and setups of simulations. ARTS is open-source software (GNU public license) implemented in C++.

ARTS’ corner stone capabilities can be summarised by:

- 1D to 3D ellipsoidal planet-atmosphere system and surface topography
- arbitrary observation geometry allowing to consider refraction
- state-of-the-art absorption models: line-by-line calculations based on HITRAN or other catalogues, various continua, improved efficiency by absorption lookup tables
scattering by clouds and other particulate media; Monte Carlo (MC) and Discrete Ordinate Iterative (DOIT) solvers available
- polarised radiative transfer calculations with up to 4 Stokes components

At start of the toolbox project, the main limitations of ARTS were:
- dedicated to Earth radiative transfer
- not suitable for shortwave radiance calculations
- no handling of active (transmitter-receiver) measurement techniques
- no polarised absorption/emission by gaseous media (but polarisation by particulate media and surface)
- local thermodynamic equilibrium (LTE) conditions only

In addition to the propagation model, a data package containing example input data for running ARTS (standard and climatological atmospheric scenarios, example single scattering data for clouds) has been available.

3.2 From Earth to Planets: Generalising the Propagation Model

A major challenge when extending radiative transfer modelling from Earth to further planets is to remove a number of assumptions on basic physical parameters made in the model itself or in the input data. This includes hard-coding of “constants” that are valid for Earth but different from planet to planet. It furthermore regards assumptions in certain algorithms and parametrisations. The most prominent one is the expression of foreign pressure broadening (and pressure induced frequency shifts) by a single parameter valid for the standard mixture of Earth “air” (79% N₂ + 21% O₂). Here, the limitation is not only in the RT model itself, but spectroscopic catalogues commonly only report these single, Earth-valid parameters (e.g., HITRAN and GEISA; the JPL catalogue does not provide these parameters at all).

ARTS has been revised for such assumptions, and modifications towards more general approaches have been made. The most important of these are:
- Pressure broadening and shifts calculated from individual contributions of the gaseous atmospheric components considering the actual atmospheric composition. In general all gases could be taken into account, but current implementation is limited to the major atmospheric components of the four considered planets: N₂, O₂, H₂O, CO₂, H₂, He.
- Format of the ARTS spectroscopic data modified to hold pressure broadening and shift parameters of the major atmospheric components.
To consider refraction of ray paths, (real part of) refractive index of the atmosphere is required. A parametrisation taking into account the major atmospheric components has been added.

Previously hard-coded isotopologue ratios now have to be provided by the user. A set of ratios valid for Earth remains to be built in to the model, because needed when using HITRAN data.

Constants like the gravitational constant, molar mass of “air”, planet radius and eccentricity have to be provided by the user. Methods providing default values for a specific planet have been implemented.

3.3 Active measurement methods

For simulating active measurements, a number of features and algorithms have been newly implemented. The most important of them are:

- Algorithm for determination of two-side-bounded (transmitter-to-receiver) propagation paths allowing arbitrary positions (on ground, in or above atmosphere) of transmitter and receiver in 1D to 3D atmosphere.
- Module for radio link calculations covering a range of possible output parameters including atmospheric attenuation, defocusing, extra path delay, bending angle and impact parameter. The calculations share a wide range of functionality with passive measurement simulations (e.g., ray tracing, attenuation calculations, refraction effects, etc.).
- Capability to handle effects of free electrons, i.e., electron-induced refraction and Faraday rotation. Both can be considered in passive and active measurements (but are relevant mostly for the latter).

In parallel to the toolbox project, a simple method for simulation of backscattering radar observations (cloud radars) has been added.

3.4 Further implementations

A couple of further extensions or new developments were necessary and have been implemented:

- Infrastructure for wind, magnetic fields (both described by up to three vector components), and electron densities.
- Doppler effect due to winds and due to planet rotation can be modelled.
- Revised and extended data output mechanism allowing a wider set of possible output parameters (depending on calculation module applied) and reporting of specific parameters decomposed along the path.
Additional scattering solver, the Fixed Order of Scattering (FOS) method with choice to neglect scattering (but consider absorption/emission by particles) or to consider single scattering (neglect multiple scattering). The method allows for calculation of Jacobians. It also performs better than MC and DOIT in case of optically thin, weakly scattering atmospheres like Mars. FOS is still under development, single scattering and Jacobians options are to be used with care.

Algorithms handling Zeeman effect and line mixing are developed in parallel to the toolbox project and available to the toolbox user (not completely implemented and extensively tested yet, hence to be used with care).

ARTS is provided with a set of test cases. These ensure consistency of the model, and corresponding control files serve as setup examples for the different calculation types. Specific demo cases have been developed for the toolbox to support users with little experience of ARTS usage. These cases include passive clearsky and cloud observation setups as well as radio occultation cases for the different planets, and cases demonstrating usage of 3D data and RT for passive observations and link budgets in 3D space. All setups are done in form of easy-to-modify templates. For example, the user can select atmospheric scenario and absorbing species from a list of all available data.

3.5 Data collection

The collection of input data for ARTS has been largely extended for the toolbox. It now includes:

- spectroscopic data: a spectroscopic line catalogue suitable for absorption calculations in atmospheres of arbitrary composition as well as collision induced absorption continuum data,
- atmospheric scenarios for the considered planets: fields of temperature, gas volume mixing ratio, wind, electron density, magnetic field, cloud/haze/dust (number density),
- planet surface properties: temperature, refractive index, topography,
- single scattering properties of clouds, hazes, dust as occurring on the considered planets.

4 Results and conclusions

Implementation resulting from the project has been summarised above. Here we present selected examples of applications possible with the toolbox. All examples are taken from toolbox validation calculations.
4.1 Planetary spectra

Spectra of planetary brightness temperatures (1 MHz–3 THz) of Venus, Mars, and Jupiter have been modelled. Assuming that nadir pencilbeam simulations are representative for the full field-of-view over the disk, the simulated spectra have been compared to measurements of planetary disk brightness. This assumption is precarious as, depending on optical thickness of the atmosphere and surface reflection properties, systematic differences between full-disk and (nadir) pencilbeams spectra can occur.

Fig. 1 (left panel) shows modelling results for Venus in comparison to disk brightness observations along with their associated measurement uncertainty. At wavelengths up to about 100 mm, model and observations agree within measurement uncertainties. Increasing deviations at longer wavelengths, where modelled spectra do not reproduce the brightness temperature decrease seen in observations, are likely due to noticeable limb effects neglected by applying the nadir-pencilbeam assumption. Equivalent comparisons have been done for Jupiter and are presented in Fig. 1 (right panel). Model and measurements are in good agreement, particularly around the “ripple” structure at 0.1–0.3 mm.

For Mars, optical thickness of the atmosphere is low and surface temperature fluctuates greatly over daytime and seasons. Hence, planet brightness strongly varies making it unsuitable for validation of the propagation model. Limb observations are more suitable, but no microwave limb measurements have been performed so far. Instead, we compared to synthetic spectra of the Far-InfraRed Experiment (FIRE) (Kasai et al., 2012) simulated with an
independent model, AMATERASU (Baron et al., 2008). Results are shown in Fig. 2.

Observed deviations are mainly resulting from differences in the applied spectroscopic parameters. As spectroscopy for non-Earth conditions is quite badly known, it is impossible to prove which choice of parameter values is (more) correct. We are, however, confident that the toolbox catalogue data is the better option, as it relies on measured or individually adapted parameters, not on merely rescaled Earth-applicable data.

For Venus, Mars, and Earth, the toolbox also contains cloud and dust data. For selected scenarios, their effects on planet brightness have been modelled. In general, the influence is small for most of the particle bulks considered in the toolbox. Exceptions are Earth ice clouds, volcanic ash clouds observed close to their source, and (precipitating) Martian CO$_2$ ice clouds.

4.2 Radio link budgets

During this project, capabilities to model radio link measurements have been added to the ARTS model. Bending angles are one of the observed parameters. They are an integrated measure of the refractive index in the atmo-
sphere traversed by the ray, which in turn depends on the atmospheric composition along the ray. Refraction is affected by both the neutral atmosphere as well as by free electrons abundant in the ionosphere of planets.

Fig. 3 (left panel) shows a comparison of bending angles and tangent altitudes as modelled with ARTS and by ECMWF forward model operator in the lower (neutral) atmosphere. The agreement between the two models is in general excellent. Calculations of ionospheric bending by free electrons is presented in Fig. 3 (right panel) for Venus atmosphere. The comparison data from Imamura et al. (2011) is based on idealised data, while ARTS is taking input data from the toolbox data package. The basic shapes of the two bending angle profiles are very similar, including the magnitude of the negative peak value.

ARTS also provides received power and contributions of the different attenuation mechanisms to the transmission. Fig. 4, left panel, shows ARTS and GRAS bending angles, while right panel illustrates the relative importance of the attenuation mechanisms for Earth radio occultations. GRAS and ARTS relative powers agree in the general vertical variation. This is not always the case, but this can be accounted to instabilities in the recorded power.
Figure 4: Comparison of ARTS calculations with GRAS data. The input to ARTS is data retrieved by ECMWF from the GRAS bending angles.

4.3 Wind Doppler shifts

Many microwave forward models do not account for wind induced Doppler shifts. The new ARTS implementation has been compared to the model presented by Baron et al. (2013). Results are shown in Fig. 5 for a simulation of the 183 GHz water vapour line. The models predict very similar wind induced changes of the spectra with deviations between the models in the order of 1%.

5 Recommendations

In general, ARTS can be applied for calculations in the thermal IR spectral range. The accuracy of calculations for non-Earth planets is limited by the available spectroscopic data. For the toolbox, planet-suitable spectroscopic data has been collected up to sub-millimetre frequencies only. It would be very valuable to extend the line database to the IR spectral range. Even

Figure 5: Results from wind Doppler comparison. (left) Simulated spectra. (middle) Deviation to simulation with no wind (ARTS results as black crosses). (right) Deviation between the models for wind effects.
better would be if the newly established reporting scheme of pressure broadening and shift parameters (per individual species instead of per mean “air”) could propagate into established catalogues.

A crucial upcoming application area of the ARTS model is the simulation of cloud-affected sub-millimetre radiances by the ICI and MWI sensors on Metop-SG. This requires extensive development work in the handling of hydrometeor input parameters (mapping of 3D fields of liquid water and ice water content, optionally also of further moments of the particle size distribution, to single scattering parameters). It also requires a more efficient scattering radiative transfer solver, since the ones currently implemented in ARTS, while accurate, are too slow for this application. To support the ICI/MWI missions, the community needs an accurate and fast forward operator translating detailed cloudy atmospheric model states to simulated satellite measurements. Available tools like RTTOV only partly fulfil these requirements, since they do not treat all aspects of these new missions, particularly not polarisation effects due to cloud scattering. We therefore recommend a dedicated ESA study to develop an ICI/MWI RT toolbox, similar to the planetary toolbox, but focused on these upcoming missions for Earth’s atmosphere.

For modelling line mixing and Zeeman splitting effects, which are relevant for Earth as well as other planets, the stage has been set within ARTS, but further developments and improvements as well as careful testing are necessary. Local thermodynamic equilibrium (LTE) conditions that are currently assumed throughout the toolbox break down in atmospheric regions of low pressure, e.g., in thin atmospheres like of Mars or the Jovian moons, but also the upper atmosphere of Earth. Extending the toolbox to handle non-LTE conditions is desirable.

For radio link calculations, an alternative set of propagation path functions should be set up, where the division of the path into steps is avoided. This would improve calculation speed, and potentially also decrease the sensitivity to numerical issues. Speed and stability could also be improved by implementing an Abel transform based simulation method.

Further desirable modifications regard improved user-friendliness and easier usage of the model for specific applications. Simulations of satellite observation sequences could be facilitated by methods that map orbital parameters to receiver positions, satellite velocity vector and other data of similar type. Also, considering polarisation effects when performing simulations of full disk observations is currently is complicated, but could be eased by development of suitable sensor methods.
References


