

Atmospheric radiative transfer generalized for use on Earth and other planets: ARTS 2.2



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Contents

Background

"Planetarization" adaptations

- Ine modeling approach
- refractivity
- isotopologue ratios
- ► CIA
- planet parameters
- Further new ARTS features
- Data collection

Summary



- theory and implementation
- user-interface

Background

- increasing interest in RT modeling for planet atmospheres
- sophisticated Earth RT models available, e.g. ARTS
- conditions on planets are different, i.e. adaptations required
 - specialised RT models (planet, spec. region)
 - ▶ generalized planetary model ⇒ consistency!



Background

- triggered by ESA project "Microwave propagation toolbox for planetary atmospheres"
 - Earth, Venus, Mars, Jupiter
 - frequencies <3THz</p>
 - propagation modeling (passive+active) + data
- our solution approach: revise & generalize ARTS



- common implicit assumptions (strictly) valid for Earth only
 - ▶ air = 79% N2 + 21% O2
 - parameters expressed in terms of (ambient) total pressure
- remove assumptions:
 - apply actual atmospheric composition
- allow to use and set planetary parameters for currently considered planet
- extend data to cover planetary conditions, e.g., continua



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expressed in terms of total pressure:

- foreign pressure broadening
- pressure shift
- the common formulation:

$$\gamma_L = x_{\text{self}} p \text{ SGAM} \left(\frac{\text{T}_{\text{GAM}}}{T}\right)^{\text{NSELF}} + (1 - x_{\text{self}}) p \text{ AGAM} \left(\frac{\text{T}_{\text{GAM}}}{T}\right)^{\text{NAIR}}$$



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replace by formulation in terms of species-specific contributions

the common formulation:

$$\gamma_L = x_{\text{self}} p \text{ SGAM} \left(\frac{\text{T}_{-}\text{GAM}}{T}\right)^{\text{NSELF}} + (1 - x_{\text{self}}) p \text{AGAM} \left(\frac{\text{T}_{-}\text{GAM}}{T}\right)^{\text{NAIR}}$$

the revised formulation:

$$\gamma_{L} = x_{\text{self}} p \text{ SGAM} \left(\frac{T_I0}{T}\right)^{\text{NSELF}} + (1 - x_{\text{self}}) p \frac{\sum_{i} \left[x_{i} \text{ GAMMA}_{i} \left(\frac{T_I0}{T}\right)^{N_{i}}\right]}{\sum_{i} x_{i}}$$

- some practical (implementation) issues
 - species-specific broadening/shift contributions implemented for limited set of species
 - model atmosphere allows total VMR<1</p>



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⇒rescale foreign broadening such that VMR_{total(broad.spec.).}=1

$$\gamma_{foreign} = (1 - VMR_{self}) p \cdot \sum_{i=broad.spec.} \gamma_i / \sum VMR_i$$

ensures consistency with "classical" approach



from the user side:

- ► nothing specific to do by the user ☺
- applied approach is determined by format of applied line catalogue (or the individual line record!)
- classical and new approach can be applied in parallel
- Ine catalogue files carry format tag
- reading routine is adaptive



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```
<?xml version="1.0"?>
                                                         <?xml versit
                                                         <arts format="ascii" version="1">
<arts format="ascii" version="1"
                                                         <ArrayOfLineRecord version="ARTSCAT-4" nelem="3">
<ArrayOfLineRecord version="ARTSCAT-3" nelem="1">
@ O-6 2060067944638.33 0 2.87793884119732e-16 296
                                                            HF-19
                                                                       1232476234457.38 0.29624E-11 296
                                                                       2370935635414.22 0.76459E-19 296
</ArrayOfLineRecord>
                                                            HF - 19
                                                                                                          0...5
</arts>
                                                            HF-19
                                                                       2463428114203.56 0.17631E-10 296
                                                                                                          8.0
                                                         </ArrayOfLineRecord>
                                                         </arts>
```

- reading routine is adaptive
- classical and new approach can be applied in parallel

Planet Adaptations – Line catalogue

generalized line modeling requires

- extended set of spectroscopic parameters
- revised line catalogue format
- newly compiled line catalogue
 - here: for f<3THz, from literature</p>
 - in future: extended-database-HITRAN



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Planet Adaptations – Catalogue format

► old format (ARTSCAT-3):

similar to HITRAN, but less restricted format

Col	Variable	Label	Unit
0	,6,	ENTRY	
1	molecule & isotopologue tag	NAME	-
2	center frequency	F	Hz
3	pressure shift of F	PSF	Hz/Pa
4	line intensity per molecule	ΙO	m^2/Hz
5	reference temp. for IO	T_IO	K
6	lower state energy	ELOW	J
7	air broadened width	AGAM	Hz/Pa
8	self broadened width	SGAM	Hz/Pa
9	AGAM temp. exponent	NAIR	-
10	SGAM temp. exponent	NSELF	-
11	ref. temp. for AGAM, SGAM	T_GAM	K
12	number of aux. parameters	N_AUX	-
13	auxiliary parameter	AUX1	-
14			
15	error for F	DF	Hz
16	error for IO	DIO	9
17	error for AGAM	DAGAM	00
	error for SGAM	DSGAM	90 00
	error for NAIR	DNAIR	90 10
	error for NSELF I	ONSELF	8
The Atmospheric Radiative Tra	error for PSF	DPSF	00

Planet Adaptations – Catalogue format

- planet generalized format(ARTSCAT-4):
 - needs to hold further parameters (speciesspecific broadening & shift information)

1		2
the	ADTC	2
	ARIS	2
WE SHILL	/	2
HUH-	The Atmospheric Radiative Tra	2
		-

Col	Variable	Label	Unit
0	`@'	ENTRY	
1	molecule & isotopologue tag	NAME	-
2	center frequency	F	Hz
3	line intensity	IO	Hz*m^2
4	reference temperature	T_I0	K
5	lower state energy	ELOW	J
6	Einstein A-coefficient	А	1/s
7	Upper state stat. weight	G_upper	-
8	Lower state stat. weight	G_lower	-
9	broadening parameter self	SGAM	Hz/Pa
10	broadening parameter N2	GAMMA_N2	Hz/Pa
11	broadening parameter O2	GAMMA_02	Hz/Pa
12	broadening parameter H2O	GAMMA_H2O	Hz/Pa
13	broadening parameter CO2	GAMMA_CO2	Hz/Pa
14	broadening parameter H2	GAMMA_H2	Hz/Pa
15	broadening parameter He	GAMMA_He	Hz/Pa
16	GAM temp. exponent self	NSELF	-
17	GAM temp. exponent N2	N_N2	-
18	GAM temp. exponent O2	N_02	-
19	GAM temp. exponent H2O	N_H2O	-
20	GAM temp. exponent CO2	N_CO2	-
21	GAM temp. exponent H2	N_H2	-
22	GAM temp. exponent He	N_He	-
23	F pressure shift N2	DELTA_N2	Hz/Pa
24	F pressure shift O2	DELTA_02	Hz/Pa
25	F pressure shift H2O	DELTA_H2O	Hz/Pa
26	F pressure shift CO2	DELTA_CO2	Hz/Pa
27	F pressure shift H2	DELTA_H2	Hz/Pa
28	F pressure shift He	DELTA_He	Hz/Pa
29	Vib. & rotational assignment	s VRA	_

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neutral gaseous atmosphere

commonly parametrized in terms of total pressure, e.g.

$$(n-1) \times 10^{\circ} = N = 77.6(P_a/T)Z_a^{-1} +$$

(Thayer74)

now: treat each species as separate contributor

additionally: free electron contribution



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 $N = N_{\text{ref},1} \frac{n_1}{n_{\text{ref},1}} + N_{\text{ref},2} \frac{n_2}{n_{\text{ref},2}} + \dots = \frac{273.15 \,\text{K}}{760 \,\text{Torr}} \left[N_{\text{ref},1} \frac{p_1}{T} + N_{\text{ref},2} \frac{p_2}{T} + \dots \right]$

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from the user side:

- different approaches implemented as workspace methods
- air refractive index provided by an agenda, used defines which methods/settings to apply:

pre-defined agendas provided (in agendas.arts), user just needs to copy the desired one.

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```
***
# Combination of Thayer + free electrons. OK for Earth and microwave.
                                        ###
AgendaSet( refr index air agenda ){
                                        # combined refraction from gases (Newell&Baird) and free electrons
  NumericSet( refr index air, 1.0 )
                                        # valid for arbitrary planetary atmospheres in microwave
 NumericSet( refr index air group, 1.0 )
 refr index airThayer
                                        AgendaSet( refr index air agenda ){
 refr index airFreeElectrons
                                          NumericSet( refr index air, 1.0 )
                                          NumericSet( refr index air group, 1.0 )
                                          refr index airMWgeneral
                                                                      ***
                                          refr index airFreeElectrons
                                                                     # no refraction (n==1.0)
                                                                     AgendaSet( refr index air agenda ){
                                                                        Ignore( f grid )
           pre-defined agendas provided
                                                                       Ignore( rtp pressure )
                                                                       Ignore( rtp temperature )
              (in agendas.arts), user just needs
                                                                       Ignore( rtp vmr )
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 - required as HITRAN line strengths are scaled with isotopologue ratio
 - "in code" from HITRAN (where available), i.e., reflecting Earth conditions
 - ⇒ impractical to remove these from code



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 - ► can be set from built-in set of ratios (⇒ Earth)
 - ► can be read from file (⇒ planets)
 - files with isotopologue ratio data for each planet are part of the toolbox data package
 - from modified D/H (all) and 15N/14N (Mars, Jupiter); others (13C/12C, 18O/16O, 17O/16O) within 5% of Earth

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```
<?xml version="1.0"?>
<arts format="ascii" version="l">
<SpeciesAuxData version="1" nelem="204" nparam="1">
# H20-161 0.997572947934
 H20-181 0.00200034318924
 H20-171 0.000372095461312
# H2O-162 5.23649842028e-05
# H20-182 1.05002501676e-07
# H2O-172 1.95261577018e-08
# H20-262 6.37002016557e-10
8 H2O-SelfContStandardType nan
8 H2O-ForeignContStandardType nan
# H2O-ForeignContMaTippingType nan
 H2O-ContMPM93 nan
 H2O-SelfContCKDMT100 nan
 H2O-ForeignContCKDMT100 nan
6
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6

- ARTS offers plenty of continuum models
- for Earth, though (either empirical models or pressure parametrised with fix-air assumption)
- atm. conditions are different on other planets
 incl. Venus and Jupiter with high pressures
- (completely) different species have significant continuum absorption
- implemented new continua
 - namely HITRAN CIA data



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implemented HITRAN CIA data

Temperature: 310 K, partial pressure of each gas: 1000 hPa 10⁻²⁷ N2-CIA-N2-0, N2-CIA-N2-1 N2-CIA-H2-0 N2-CIA-CH4-0 H2-CIA-H2-0 Abs. Cross-section [m² molec⁻¹] H2-CIA-He-0 H2-CIA-CH4-0 02-CIA-02-0 CO2-CIA-CO2-0 CH4-CIA-CH4-0 CH4-CIA-Ar-0 10⁻³⁰ L 1000 1500 500 2000 2500 0 Wavenumber [cm⁻¹] RTS The Atmospheric Radiative Transfer Simulator

⇒implemented HITRAN CIA data

species Temperature: 310 K, partial pressure of each gas: 1000 hPa 10⁻²⁷ N2-CIA-N2-0, N2-CIA-N2-1 N2-CIA-H2-0 N2-CIA-CH4-0 H2-CIA-H2-0 Abs. Cross-section [m² molec⁻¹] Jupiter atmosphere @ p=1.00e+04Pa H2-CIA-He-0 10-2 C2H2 H2-CIA-CH4-0 10-5 C2H4 02-CIA-02-0 10-8 C2H6 CO2-CIA-CO2-0 10-11 C3H8 CH4-CIA-CH4-0 [1/m] 10⁻¹⁴ CH4 CH4-CIA-Ar-0 10⁻¹⁷ CO2 coefficients CO 10⁻²⁰ H2 10⁻²³ 10⁻²⁹∟ H2S 10⁻²⁶ He extinction 10⁻²⁹ PH3 H2-CIA-H2-0 10⁻³² H2-CIA-He-0 10-35 H2-CIA-CH4-0 10⁻³⁸ CO2-CIA-CO2-0 10-41 CH4-CIA-CH4-0 -30 10⁻⁴⁴ 10

500

1000

1500

Frequency [GHz]

2000

1000 500 1500 2000 2500 Wavenumber [cm⁻¹] ARTS

0

ARTSworkshop 2014 jana.mendrok@ltu.se

2500

3000

other planets ⇒ other

significant continuum

The Atmospheric Radiative Transfer Simulator

⇒implemented HITRAN CIA data

10⁻²⁷

Abs. Cross-section [m² molec⁻¹]

10⁻²⁹∟

-30

0

10

significant continuum species Temperature: 310 K, partial pressure of each gas: 1000 hPa N2-CIA-N2-0, N2-CIA-N2-1 N2-CIA-H2-0 N2-CIA-CH4-0 H2-CIA-H2-0 Jupiter atmosphere @ p=1.00e+04Pa H2-CIA-He-0 10-2 C2H2 H2-CIA-CH4-0 10-5 C2H4 02-CIA-02-0 10-8 C2H6 CO2-CIA-CO2-0 10-11 C3H8 CH4-CIA-CH4-0 [1/m] 10⁻¹⁴ CH4 CH4-CIA-Ar-0 10⁻¹⁷ CO2 coefficients CO 10⁻²⁰ H2 10⁻²³

10⁻²⁶

other planets ⇒ other

H2S

He

extinction 10⁻²⁹ PH3 10⁻³² H2-CIA-H2-0 H2-CIA-He-0 10⁻³⁵ H2-CIA-CH4-0 10⁻³⁸ CO2-CIA-CO2-0 10-41 CH4-CIA-CH4-0 10⁻⁴⁴ 500 1000 1500 2000 2500 3000 1000 500 1500 2000 2500 Frequency [GHz] Wavenumber [cm⁻¹] some data gap issues ARTS ARTSworkshop 2014 The Atmospheric Radiative Transfer Simulator jana.mendrok@ltu.se

- planet size and shape
- sidereal rotation period
- molar mass of dry air
- gravity constant



planet size/shape:

set manually from "basic" workspace method:

```
refellipsoidSet( refellipsoid, re, e )
```

set by planet-specific workspace methods ("model" choices: sphere or ellipsoid):

refellipsoidMars(refellipsoid, model)



explicitly manually set numeric:

- sidereal rotation period
- molar mass of dry air
- gravity constant
 - set by agenda (g0_agenda)
 - apply planet-specific workspace methods:
 g0Mars(g0)
 - alternatively, set numeric manually



- as support for the user, include file for each planet provided
 - controlfiles/general/planet_XXX.arts

performing the settings for:

- isotopologue ratios
- reference ellipsoid (only as sphere, though!)
- gravity
- sidereal rotation period
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New features

- active measurement techniques
 - radio link budgets, radio occultation
 - transmitter-receiver-path ray tracing
- Doppler shifts
 - wind, planet rotation, (sensor movement)
- polarized gas absorption
 - Zeeman splitting, Faraday rotation
- extended atmospheric characterization
 - magnetic field, electron density, wind
- Dispersion
- n²-law of radiance
- auxiliary output

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New features – atmosphere

- new absorption species free_electrons
- electron density as vrm_field entry
- grid conversion by AtmFieldsCalc
- additional workspace variables
 - wind_u/v/w_field
 - > mag_u/v/w_field
- explicit grid conversion of raw data required: GriddedFieldPRegrid, GriddedFieldLatLonRegrid



New features – Doppler

wind Doppler

- no user action required
- considered when any of wind_u/v/w_field non-zero
- horizontal winds (v/u) require 2D/3D
- planet rotation
 - modelled as pseudo-wind
 - via WSM wind_u_fieldIncludePlanetRotation
- wind Jacobians possible



New features – Faraday

- via WSM propmat_clearskyAddFaraday
 - e.g. as part of propmat_clearsky_agenda
- requires
 - absorption species free_electrons
 - mag_u/v/w_field being non-zero



New features – transmitter-receiver

- required for active meas. techniques
- direct path (!)
- specified by position
 - transmitter (transmitter_pos/rte_pos2)
 AND
 - receiver (sensor_pos/rte_pos)
- performed by applying ppathFromRtePos2 in ppath_agenda



New features – Auxiliary output

- intermediate variables that are usually not accessible on ARTS controlfile level, e.g.
 - along-LOS parameters: (per-species) absorption, T, iy
 - derived parameters: optical depth
- different per applied RT method
 - iyCalc Or yCalc (no LOS decomp)
 - iy_main_agenda method (see built-in doc)
- Output format: ArrayOfTensor4/Vector
- selected via iy_aux_vars (array of string identifiers)

The Atmospheric Radiative Transfer Simulator

RTS

New features – n²-law

- implicitly handled by iyEmissionStandard
- no issue if
 - sensor in space (vacuum)
 - ► n_{sensor}≈1
 - output as Tb
- else: manual n² scaling by user required



New features – Dispersion

- usually, all frequencies in parallel on identical ray path (no dispersion)
- to consider dispersion:
 - set iy_main_agenda as
 - > AgendaSet(iy_main_agenda){
 iyLoopFrequencies}
 - set iy_sub_agenda
 - apply a dispersive refractive index
 - refr_index_airFreeElectrons



Data collection

- in arts-xml-data package
- spectroscopy
 - Ine catalogue, CIA data
- planet data
 - atmospheric scenarios: fields of z(p), T, VMRs, wind, N_e, B, clouds
 - surface data: e.g., T_{surf}, z_{surf}, n_{surf}
 - isotopologue ratios
- cloud optical properties



Demo cases

In controlfiles/planetary_toolbox/

- template-like demos
 - easy to adapt (?)
 - setups reflect data available with toolbox



Results examples – Planet brightness







Summary

- ARTS revised for use with non-Earth planets
 - applying generalized approaches
 - some limitations apply
 - line data for f<3THz only</p>
- extended modeling capabilities
- extended data collection

all part of newly released ARTS 2.2

