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Impact of Spectroscopic Parameter Archive on Second Generation Vertical Sounders Radiance Simulation: the GEISA/IASI Database as an example

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Abstract : - The performances of new atmospheric sounders like AIRS (Advanced InfraRed Sounder), in the USA, and IASI (Infrared Atmospheric Sounder Interferometer) in Europe, which have a better vertical resolution and accuracy, compared to the presently existing satellite infrared vertical sounders, is directly related to the quality of the spectroscopic parameters of the optically active gases. For these instruments, the so-called GEISA (Gestion et Etude des Informations Spectroscopiques Atmosphériques; Management and Study of Atmospheric Spectroscopic Information /IASI) spectroscopic sub-database has been elaborated from the general GEISA spectroscopic database system, with the specific purpose of assessing the capability of measurement by the IASI instrument, within the designated goals of ISSWG (IASI Sounding Science Working Group), in the frame of the CNES (Centre National d'Etudes Spatiales, France) /EUMETSAT (EUropean organization for the exploitation of METeorological SATellites) European Polar System (EPS) preparation.

The purpose of this paper is to show some selected results of critical assessments, in terms of spectroscopic line parameters archive. Spectroscopic parameters difference impacts are discussed in the context of comparisons between recorded and calculated experimental spectra, using the ARA (Atmospheric Radiation Analysis) /4A (Automatized Atmospheric Absorption Atlas) forward line-by-line radiative transfer modeling code in its latest version. All the archived spectroscopic data of GEISA and GEISA/IASI can be handled through a user-friendly associated management software, which is posted on the ARA/LMD group web site at: *http://ara.lmd.polytechnique.fr*

Key-Words: - spectroscopic line parameters; satellite vertical infrared sounders; GEISA; GEISA/IASI

List of Acronyms:
AIRS: Advanced InfraRed Sounder; **ARA:** Atmospheric Radiation Analysis; **4A**: Automatized Atmospheric Absorption Atlas; **CAMEX-1**: first Convection And Moisture Experiment campaign; **CNES**: Centre National d'Etudes Spatiales, France; **EPS**: European Polar System; **EUMETSAT**: EUropean organization for the exploitation of METeorological SATellites; **GEISA**: Gestion et Etude des Informations Spectroscopiques Atmosphériques/ Management and Study of Atmospheric Spectroscopic Information; **HIS**: High-resolution Interferometer Sounder; **HITRAN**: HIgh resolution TRANsmission spectroscopic database; **IASI**: Infrared Atmospheric Sounder Interferometer; **ISSWG**: IASI *S*ounding Science Working Group; **LMD**: Laboratoire de Météorologie Dynamique ; **METOP**: METeorological OPerational Satellite ; **MIPAS**: Michelson Interferometer for Passive Atmospheric Sounding; **RAL**: Rutherford Appleton Laboratory; **TIGR**: Thermodynami*c* Initial Guess Retrieval ;

1 Introduction

Line-by-line compilations of spectroscopic parameters are used for a vast array of applications and especially for terrestrial atmospheric remote sensing. Related with the radiance simulation for actual or near future atmospheric sounders, reviews of the current state and recent developments of public spectroscopic databases, such as GEISA-03 [1] and GEISA/IASI-03 [2], HITRAN-04 [3], MIPAS [4], etc… are continually made. Actually, the performance of instruments like AIRS (*http://www.airs.jpl.nasa.gov*) and IASI (*http://earth-sciences.cnes.fr/IASI/*), which have a better vertical resolution and accuracy, compared to the presently existing satellite infrared vertical sounders, is directly related to the quality of the spectroscopic parameters of the optically active gases, since these are essential input in the forward models used to simulate recorded radiance spectra.

The purpose of this paper is to present selected results of critical assessments, in terms of spectroscopic line parameters archive, in the context of comparisons between recorded and calculated experimental or simulated spectra.

2 GEISA-03 and GEISA/IASI-03 Overview

GEISA [5], [1], a computer-accessible spectroscopic database, was designed [6] to facilitate accurate and fast forward calculations of atmospheric radiative transfer using a line-by-line and (atmospheric) layer-by-layer approach. In its 2003 edition [1], GEISA-03 is comprised of three independent sub-databases devoted, respectively, to:

- ***infrared spectral line parameters,*** related with 42 molecules (98 isotopic species), corresponding to

1,668,371 entries in the spectral range from 10^{-6} to 35,877 cm^{-1} (see summary in Table 1).

- absorption cross-sections, in the spectral range of the infrared (32 molecular species, mainly CFC's) and of the Ultra Violet/Visible (11 molecular species).

- microphysical and optical properties of basic atmospheric aerosols.

The GEISA/IASI database was derived from GEISA, as described in [7]. It has been created for the purpose of assessing the capability of IASI, within the ISSWG, in the framework of the CNES/EUMETSAT EPS preparation. EUMETSAT is planning to implement GEISA/IASI into the ground segment of EPS.

The current edition, GEISA/IASI-03 [2], is both an extract, which has been devised to suit the needs of IASI or AIRS within the 599-3001 cm^{-1} spectral range from a more extensive GEISA database and a continuing update of GEISA-03 [1], with a similar structure, including three sub-databases related with:

- infrared spectral line parameters, of 14 molecules (53 isotopic species): H2O, CO2, O3, N2O, CO, CH4, O2, NO, SO2, NO2, HNO3, OCS, C2H2, N2 corresponding to 702,550 entries (see summary in Table 2).

- infrared absorption cross-sections (mainly CFC's) for 6 molecular species: CFC-11, CFC-12, CFC-14, CCl4, N2O5, HCFC-22

- microphysical and optical properties of basic atmospheric aerosol components (similar with the GEISA-03 archive) Among the 30 kinds of archived spectroscopic parameters in GEISA and GEISA/IASI (for each entry), those of first importance for radiative transfer modeling, and used in the GEISA general management associated software, are: the wavenumber (cm^{-1}) of the line associated with the rovibrational transition; the intensity of the line (cm $molecule^{-1}$ at 296K); the Lorentzian collision halfwidth ($cm^{-1}atm^{-1}$ at 296K); the energy of the lower level of the transition (cm^{-1}); the transition quantum identifications for the lower and upper levels of the transition; the temperature dependent coefficient *n* of the halfwidth.

MOLECULE	# ENTRIES	MOLECULE	# ENTRIES
H2O	58726	HF	107
CO2	76826	HCl	533
O3	319248	HBr	1294
N2O	26681	HI	806
CO	13515	ClO	7230
CH4	216196	OCS	24922
O2	6290	H2CO	2701
NO	99123	C2H6	981
SO2	38853	CH3D	35518
NO2	104224	C2H2	3115
NH3	29082	C2H4	12978
PH3	11740	GeH4	824
HNO3	171504	HCN	2550
OH	42866	C3H8	8983

Table 1: GEISA-03 individual lines sub-database content summary

MOLECULE	# TRANSITIONS
H2O	13278
CO2	50840
O3	195102
N2O	18966
CO	3674
CH4	121281
O2	435
NO	29608
SO2	22301
NO2	71687
HNO3	152586
OCS	19768
C2H2	2904
N2	120

Table 2: GEISA-03 individual lines sub-database content summary

3 GEISA-03 and GEISA/IASI-03 H2O archive update assessment

Updates occur for 10 molecules, i.e.: H2O, CO2, O3, N2O, CH4, O2, NO, NO2, NH3, PH3. In the following example is illustrated a critical evaluation of the impact of newly archived spectroscopic parameters on IASI direct sounding modeling. The computations have been processed with the current 4A-2000 version of the ARA/LMD 4A fast line-by-line model [8] [9], an advanced version of the nominal line-by-line code STRANSAC [10], relying on GEISA/IASI-03. 4A allows the fast computation of the transmittance of discrete non-scattering atmospheric layers, and of the radiance at a user defined observation level, thanks to the use of a comprehensive database (the atlases) of monochromatic optical thicknesses for up to 43 atmospheric molecular species [8]. The atlases are created once and for all by using the model, STRANSAC, in its latest 2000 version with up to date spectroscopy from the GEISA database. This concept has been developed by the Laboratoire de Météorologie Dynamique. 4A computes the optical thickness due to gaseous absorption for each atmospheric model layer and the 4A output is the

radiance spectrum in a user defined spectral domain between 10 and 3250 cm^{-1}. 4A can be used for a wide variety of atmospheric and surface conditions. A non apodized IASI apparatus function [11] has been used, with a spectral resolution of 0.25 cm^{-1}.
Two different series of updated spectroscopic parameters of H2O are available. They stem from the measurements from Ref. [12] and from the EUMETSAT/RAL archive [13]. A choice cannot been made as to a final selection until the results of validation campaigns are used to study the respective accuracies in a detailed manner. Currently, the data from Ref. [12] have been implemented in GEISA/IASI-03.

Figs. 1 illustrate an impact of differences in H2O spectroscopic data on forward modeling computations through comparisons of IASI spectrum simulations with upwelling spectral measurements made by the HIS [14] instrument (similarity in viewing geometry with IASI) during the CAMEX-1 [15] field campaign, on 29 September 1993. On the same graphic, in the spectral interval 850-900 cm^{-1} (part of IASI band-1), are plotted: left hand, the two HIS brightness temperatures as simulated by 4A-2000 with Toth's data (in green) and RAL data (in red), and right hand the brightness temperature differences between the HIS measurements and 4A-2000 modeling, using the same color codes as previously. These differences are expanding from -1.2K to 0.6 K. The largest discrepancies appear around, 850, 855, 871 and 887 cm^{-1} and present some more important spikes in the case of RAL data (especially at 887 cm^{-1})
.

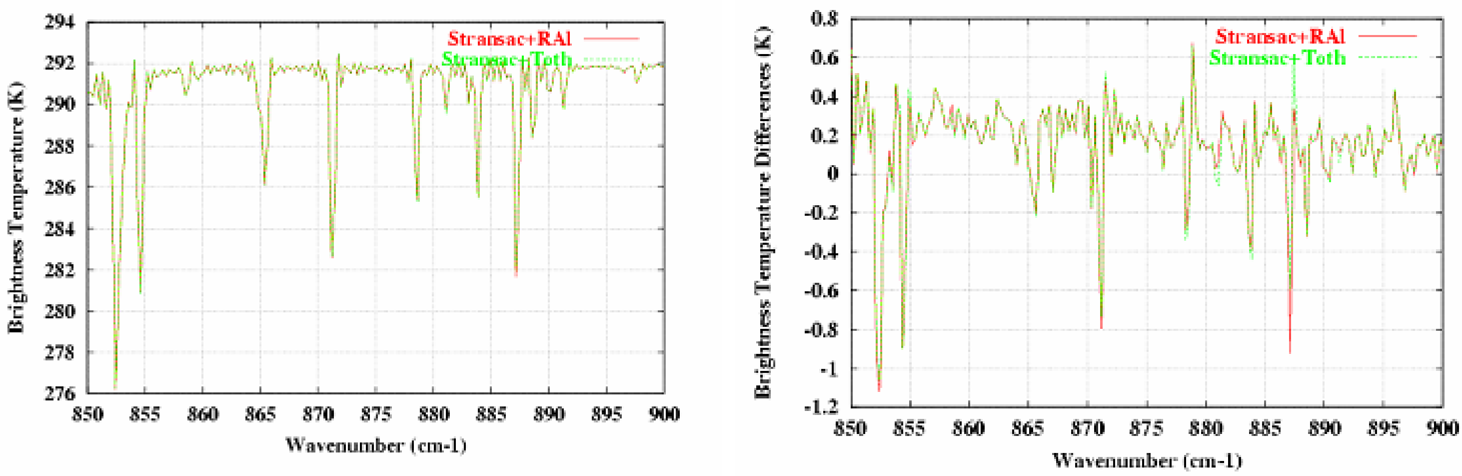
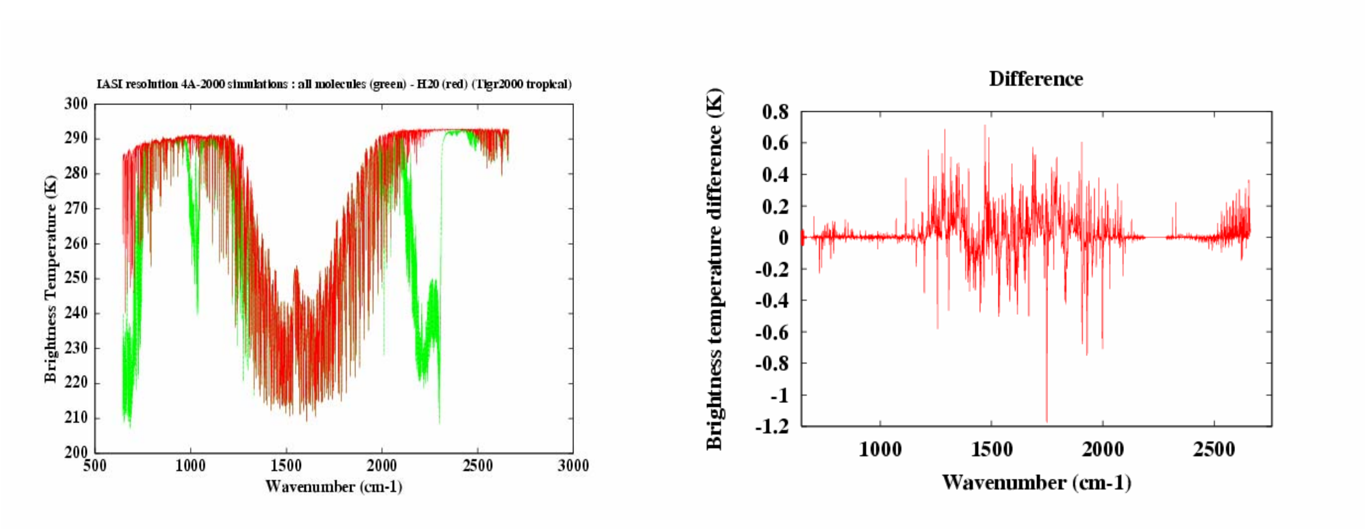


Fig 1: CAMEX(HIS) 29/09/93 campaign. Differences (ΔTB K) in 4A-2000 simulations using RAL or Toth's H2O spectroscopy in GEISA/IASI-03

4 Differences between GEISA-03 and HITRAN-04: Examples of impacts evaluation

The current editions of GEISA [1] and HITRAN, [3] exhibit differences related with the choices made for new or updated spectroscopic parameters. IASI sounding simulations have processed to evaluate impacts of these spectroscopic parameters archive differences. Computations were made in the case of a mean tropical atmospheric profile from the TIGR dataset [16-18], in its latest version (TIGR-2000).

- Fig. 2 a) shows an IASI simulation (brightness temperatures (K)) as a function of the wavenumber (IASI whole spectral range) using the GEISA/IASI-03 H2O content (in red). Related brightness temperature differences, when the original H2O data have been replaced by the HITRAN-04 ones, are on Fig. 2 b), showing spikes between nearly -1.2 and 0.8 K.



a) b)

Figs.2: GEISA/IASI-03 and HITRAN-04 H2O archive differences impact on H2O 4A-2000 IASI simulations

➢ For a TIGR-2000 tropical atmospheric situation, Fig. 3 presents IASI 4A-2000 simulations brightness temperature differences (K), for a case study related with the evaluation of the impacts of differences in spectroscopic databases archive for H2O and CH4. The red curve corresponds to the differences corresponding, either to the choice of RAL (GEISA-03(RAL) id) or to the choice of Toth's H2O data (GEISA-03 id), in GEISA/IASI -03. The green curve corresponds to the differences in using either HITRAN-04 or GEISA-03 in 4A-2000 computation. Associated with these two curves are two IASI noise curves for two temperatures: the first one (in violet) corresponds to a temperature of 280K (CNES definition [11]), and the second one (in blue) to the noise converted to the real temperature of the scene. Along the X-axis, the spectral interval is 1100-1400 cm^{-1}.

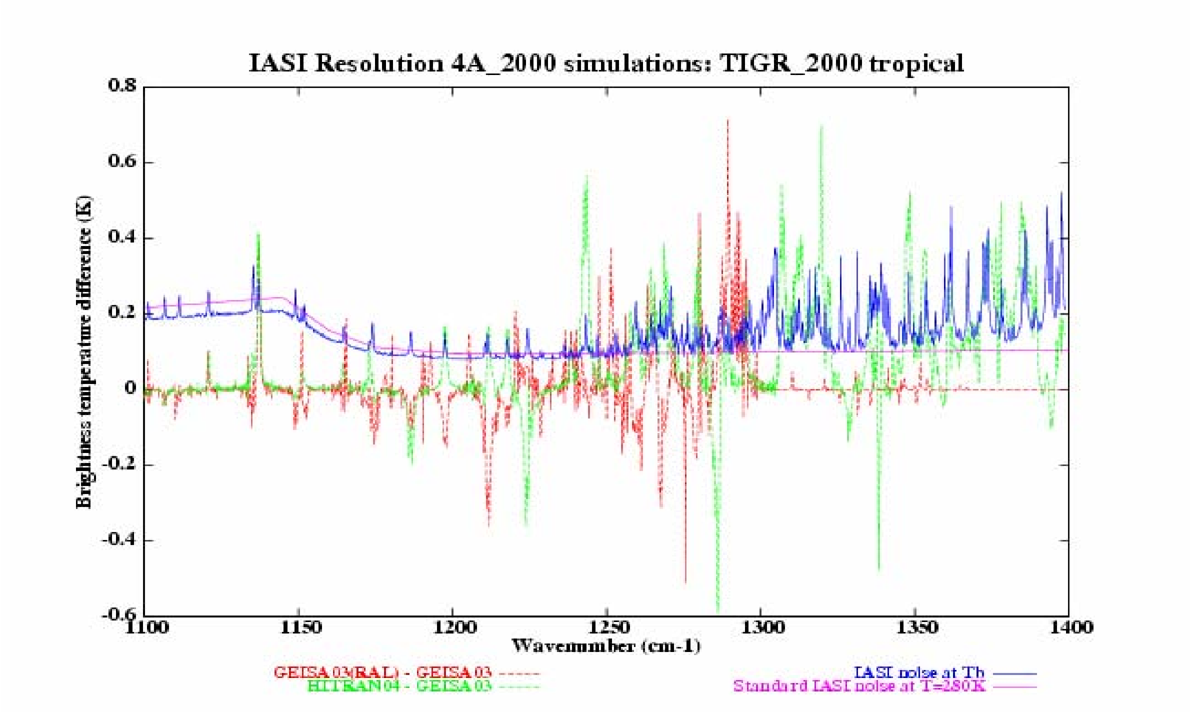


Fig.3: IASI 4A-2000 Simulations using TIGR-2000 atmospheric tropical profiles (1100-1400 cm^{-1} spectral region)

5 Conclusion

From these illustrations of IASI simulation comparisons for different archived spectroscopic parameters, it appears that the HITRAN-04 archive is significantly different from the RAL and from the Toth's/GEISA-03 one, for H2O, especially in the 1100 – 1400 cm^{-1} spectral region. Considering the actual values of IASI theoretical noise, we are confident that, when IASI real sounding data will be available, they will allow a validation in the choice of the spectroscopic parameters. For example, in the 1290 cm^{-1} spectral region, the differences between simulations, using either GEISA-03 with RAL H2O data or GEISA-03 with Toth's H2O data, show discrepancies, in brightness temperature values, of almost four times the IASI noise.

6 GEISA and GEISA/IASI management software and database availability

The GEISA management software facilities are interfaced on the ARA/LMD group web site at: http://ara.lmd.polytechnique.fr. They are also accessible at the GEISA restricted free access ftp site:http://ara.lmd.polytechnique.fr/ftpgeisa.

Previously, the potential user required a login and a password, at the ARA/LMD web site.

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