

Spectroscopic database GEISA-08 : content description and assessment through IASI/MetOp flight data



The ARA Group

The Atmospheric Radiation Analysis group is specialized in the study of the variability and evolution of the climate of the Earth from space borne observations made principally by vertical sounders, in the infrared and the microwave domains.

Its main research themes relate to the collection of a long term, global, climatology of the earth-atmosphere state: temperature and moisture; cloud characteristics, including their microphysical properties; greenhouse gases, mainly CO₂, in relation with the carbon

cycle; aerosols (volcanic, dust, smoke, etc.) infrared characteristics in relation with the earth radiative budget; continental surface infrared emissivities, in relation with the interaction between the surface and the atmosphere. The group is also deeply involved in statistical analysis of large spatio-temporal data bases (inverse problems, linear and non linear inference, neural networks, classification, pattern recognition, etc.).

The group has developed numerous tools in spectroscopy of the atmospheric gases, forward and inverse radiative transfer modelling, etc. In particular, the group develops and maintains the spectroscopic data base [GEISA](#) « Gestion et Etude des Informations Spectroscopiques Atmosphériques » (*Study and management of atmospheric spectroscopic information*).

The [Laboratoire de Météorologie Dynamique \(LMD\)](#) is a Laboratory of the French [Centre National de la Recherche Scientifique \(CNRS\)](#), of the [Ecole Polytechnique](#), of the [Ecole Normale Supérieure](#), of the [Université Pierre et Marie Curie \(Paris 6\)](#), and belongs to the [Institut Pierre-Simon Laplace \(IPSL\)](#). It is also one of the French space laboratories working in cooperation with the [Centre National d'Etudes Spatiales \(CNES\)](#).

Last update: 27th Nov 2007

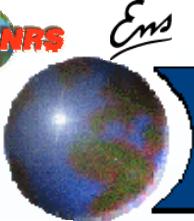
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OUTLINE

- ❖ *General Context*
- ❖ *GEISA and GEISA/IASI System Overview*
- ❖ *GEISA-08 line transition parameters sub-database*
 - 1) Database update summary
 - 2) Evaluation of the impact of H₂O spectroscopic archive differences using IASI 4A/STRANSAC Radiative transfer simulations
 - 3) Evaluation of the impact of H₂O spectroscopic archive differences using IASI Metop Flight Data and 4A/STRANSAC Radiative transfer simulations
- ❖ *Concluding Comments*



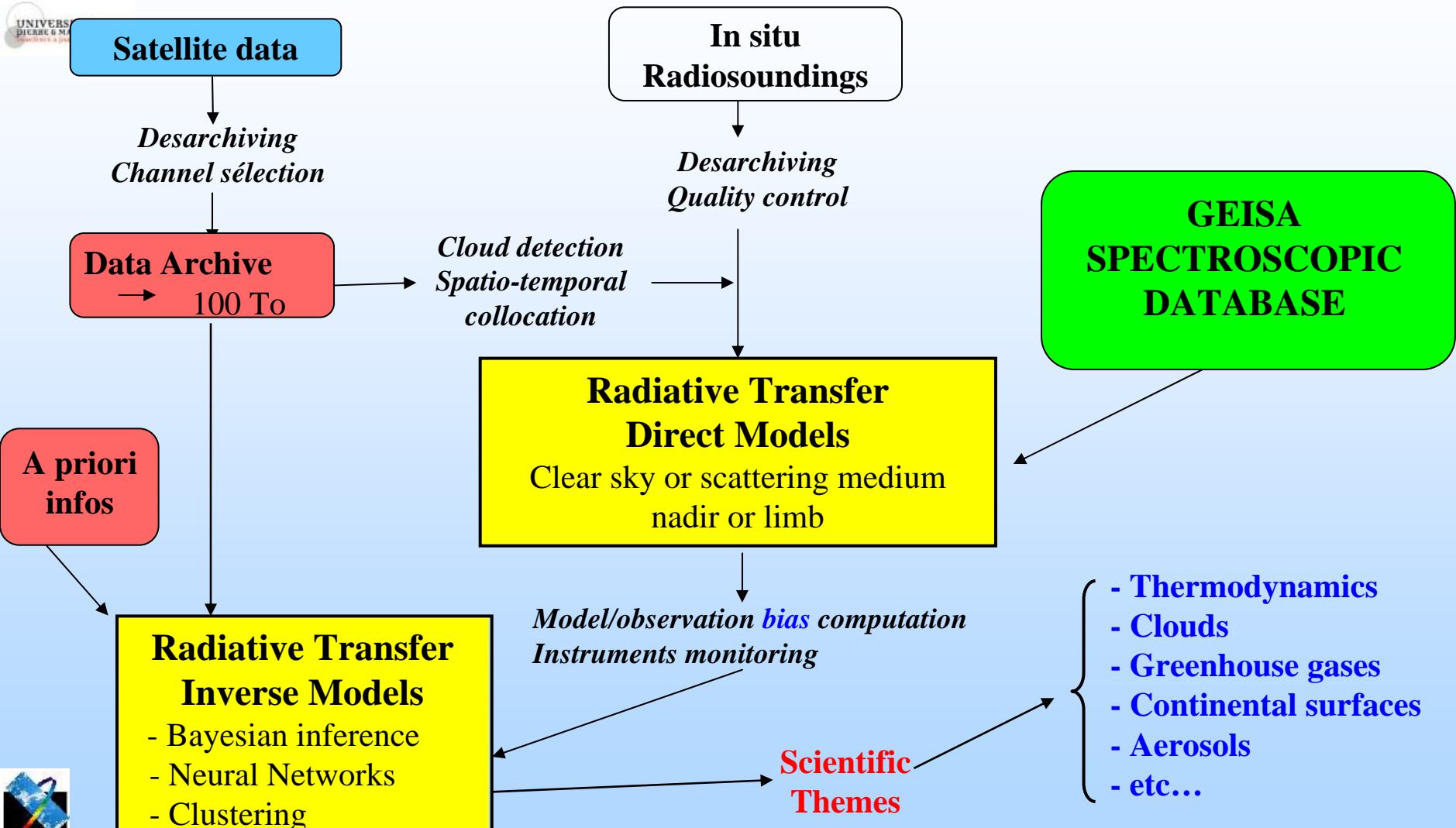
GENERAL CONTEXT



- ❖ The **ARA** (Atmospheric Radiation Analysis) group at **LMD** has been engaged, during the past three decades, in the development of **GEISA**, a computer-accessible spectroscopic database, designed to facilitate accurate and fast forward calculations of atmospheric radiative transfer using a line-by-line and (atmospheric) layer-by-layer approach.

- ❖ The performance of the second generation vertical sounding, high-resolution, sophisticated infrared spectroscopic instruments, such as **AIRS** in the USA and **IASI** in Europe, highly depends on the accuracy in the spectroscopic parameters of the optically active atmospheric gases, since such data constitute an essential input in the forward models that are used to interpret the recorded spectral radiances.

FROM SATELLITE OBSERVATIONS TO CLIMATE VARIABLES: a long process based on Radiative Transfer





42 co-authors
16 Laboratories

GEISA and

Journal of Quantitative Spectroscopy &
Radiative Transfer 95 (2005) 429–467

The 2003 edition of the GEISA/IASI spectra

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The GEISA spectroscopic database: Current and future archive for Earth and planetary atmosphere studies

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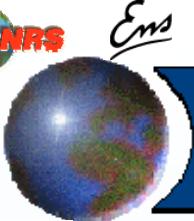
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GEISA and GEISA/IASI System Overview



THE GEISA-2008 SYSTEM

Gestion et Etude des Informations Spectroscopiques Atmosphériques
Management and Study of Atmospheric Spectroscopic Information

Three SUB-DATABASES

● Line transition parameters database

48 molecules (102 isotopic species)
over 3,200,000 entries between 0 and 35,877 cm⁻¹

● Absorption cross-sections database

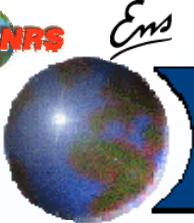
- IR: 39 molecular species (mainly CFC's)
- UV/Visible : 11 molecular species

● Aerosol data archive and softwares

ASSOCIATED MANAGEMENT SOFTWARES

(For

each sub-database)



GEISA/IASI DATABASE GENERALCONTEXT

- Extraction of GEISA-08 between 599 & 3001 cm⁻¹
 - Individual spectral lines spectroscopic parameters sub-database
14 molecules (53 isotopic species): H₂O, CO₂, O₃, N₂O, CO, CH₄, O₂, NO, SO₂, NO₂, HNO₃, OCS, C₂H₂, N₂
 - IR absorption cross-sections sub-database (mainly CFC's)
6 molecular species: CFC-11, CFC-12, CFC-14, CCl₄, N₂O₅, HCFC-22
 - Microphysical and optical properties of Basic Atmospheric aerosol components sub-database (similar with the GEISA-03 one)
- Continuous update
- Related with:
 - CNES/EUMETSAT EPS mission
 - IASI measurement capabilities assessment
 - ISSWG

Associated interest for AIRS

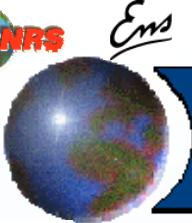
IASI : Infrared Atmospheric Sounder Interferometer

ISSWG : IASI Sounding Science Working Group

EUMETSAT : European organization for the exploitation of METeorological SATellites

AIRS : Advanced InfraRed Sounder

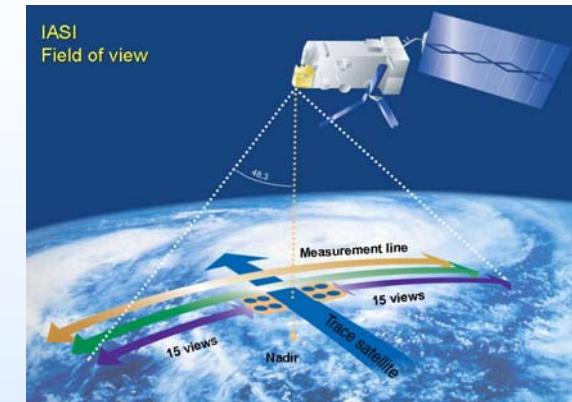
CNES : Centre National d'Etudes Spatiales, France



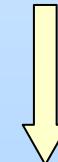
GEISA/IASI EFFECTIVE USE

IASI on METOP

since October 19th 2006 launch

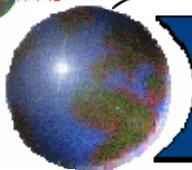


- GEISA/IASI used as the reference spectroscopic database
- Validation achieved using 4A line by line Radiative Transfer Model [Scott & Chédin, J.Appl.Met (1981); 4A/LMD <http://ara.lmd.polytechnique.fr>; 4A/OP co-developed by LMD and Noveltis with the support of CNES (2006)]



Related to

IASI Level 1 Cal/Val activities@ CNES



GEISA and GEISA/IASI interactive distribution

GEISA and associated facilities are implemented on the
Ether (CNRS/IPSL) Products and Services Centre
(CPS)

Effective January 2007

Ether Products and Services Centre Facilities:

<http://ether.ipsl.jussieu.fr>

[Welcome](#)

Welcome to the Ether website

« L'harmonieux Ether dans ses vagues d'azur enveloppe les monts d'un fluide plus pur » Lamartine

Latest news

Site

SOLSPEC : new data

ADOMOCA : version 3

REPROBUS : 2008

Community

Ether workshop : first call

Our proposal for new Ether activities

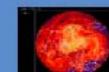
Appel_a_projet_Ether.doc

This website offers various products of French activities in national and international projects . The access rights vary according to the products (see "Login Request"). [More information ...](#)

Original products



IASI : french activities



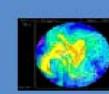
MIMOSA : Potential vorticity and temperature analysis and forecasts in Northern, Southern Hemisphere and Tropics



NDACC-FRANCE: Network for Detection of Atmospheric Composition Change



GEISA : spectroscopic data



REPROBUS : Chemistry Transport Model in Polar winters



ECCAD : data for emissions calculation



ARLETTY : temperature and pressure profiles calculation



Chemical Kinetics Database

ODIN-SMR : official data and specific production (O₃, CO, ...)

GIRAFE : biomass burning plumes

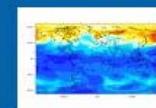


SOLSPEC : solar radiation spectrum data

Other products



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Models and Assimilations



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GEISA-08 line transition parameters sub-database

1) Database update summary

Molecular species in the GEISA individual spectral lines sub-database

- Major Permanent constituents of EARTH's atmosphere :

$O_2, H_2O, CO_2 \dots$

- Minor permanent constituents of the EARTH's atmosphere :

$O_3, CH_4, N_2O, CO \dots$

- Trace molecules in the EARTH's atmosphere :

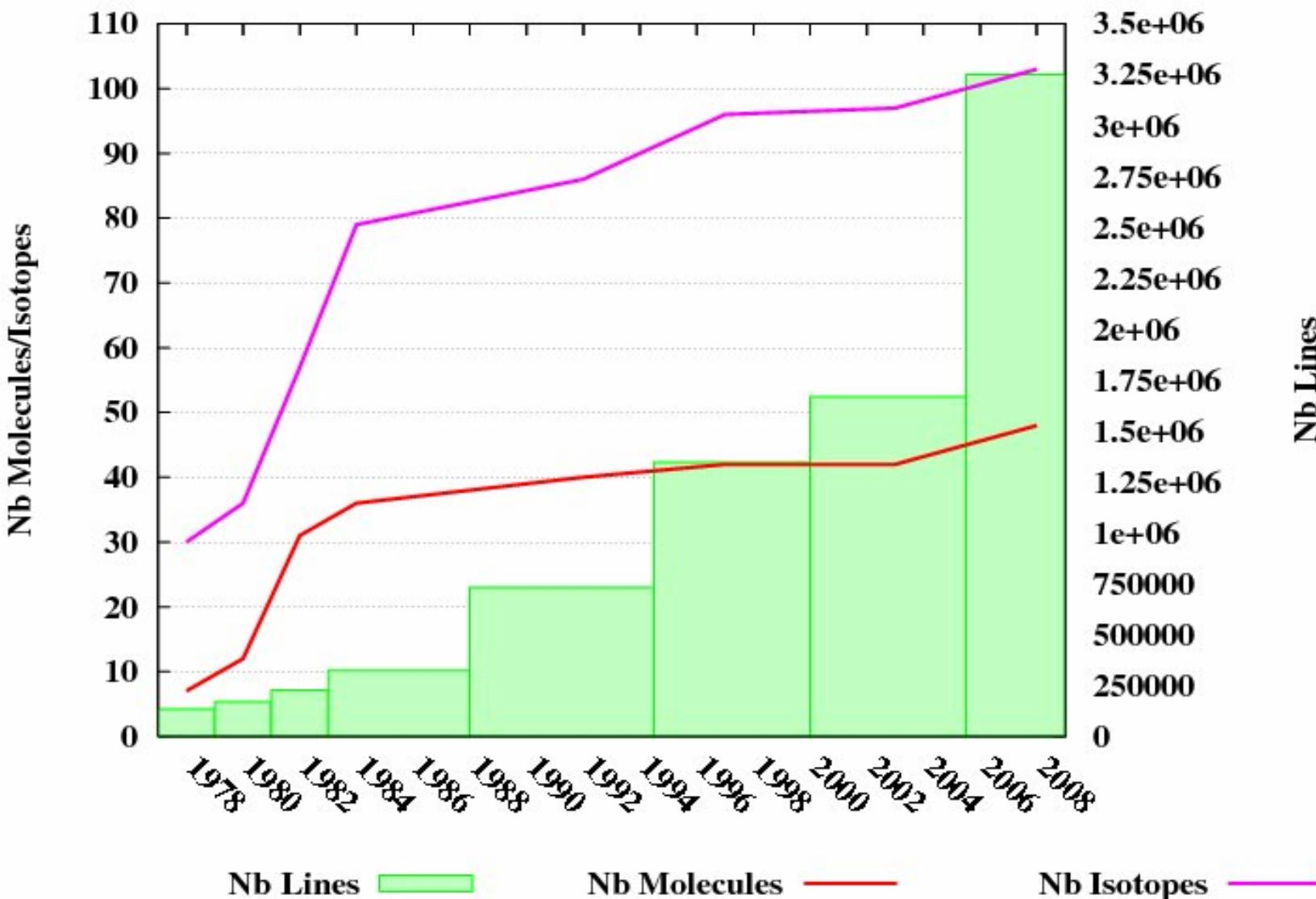
$NO, SO_2, NO_2, NH_3, HNO_3, OH, HF, HCl, HBr, HI, ClO, OCS, H_2CO, PH_3 \dots$

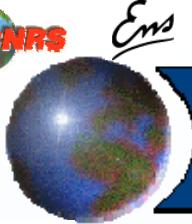
- Molecules present in the atmospheres of JUPITER, SATURN, URANUS, TITAN etc. :

$C_2H_6, CH_3D, C_2H_2, C_2H_4, GeH_4, HCN, C_3H_8, C_3H_4 \dots$

Spectral range: 0 – 35,877 cm⁻¹

EVOLUTION GEISA SINCE 1978: line transition sub-database





GEISA and GEISA/IASI-08 Line Transitions Records

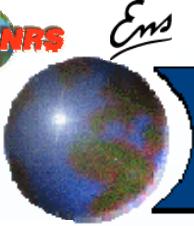
255 Characters record

30 Parameters

- (A) Wavenumber (cm^{-1}) of the line associated with the vibro-rotational transition.
- (B) Intensity of the line (cm molecule^{-1} at 296K).
- (C) Lorentzian collision halfwidth ($\text{cm}^{-1} \text{atm}^{-1}$ at 296K).
- (D) Energy of the lower transition level (cm^{-1}).
- (E) Transition quantum identifications for the lower and upper levels of the transition
- (F) Temperature dependence coefficient n of the halfwidth
- (G) Identification code for isotope.
- (I) Identification code for molecule.
- (J) Internal GEISA code for data identification.

K-Q fields mainly HITRAN inter-compatibility related

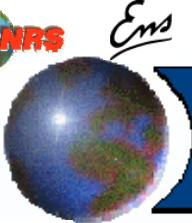
- (K) Molecule number as in HITRAN
- (L) Isotope number as in HITRAN
- (M) Einstein A-coefficient
- (N) Self broadening pressure halfwidth (HWHM) ($\text{cm}^{-1}\text{atm}^{-1}$) at 296K
- (O) Air pressure shift of the line transition ($\text{cm}^{-1}\text{atm}^{-1}$) at 296K
- (P) Accuracy indices for wavenumber, intensity and halfwidth
- (Q) Uncertainty indices



GEISA and GEISA/IASI-08 Line Transitions Records (following)

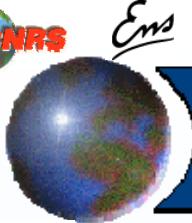
- (R) Temperature dependence coefficient n of the air pressure shift
 - (A') Estimated accuracy (cm^{-1}) on the line position
 - (B') Estimated accuracy on the intensity of the line in ($\text{cm}^{-1}/(\text{molecule.cm}^{-2})$)
 - (C') Estimated accuracy on the air collision halfwidth (HWHM) ($\text{cm}^{-1}\text{atm}^{-1}$)
 - (F') Estimated accuracy on the temperature dependence coefficient n of the air broadening HW
 - (O') Estimated accuracy on the air pressure shift of the line transition ($\text{cm}^{-1}\text{atm}^{-1}$) @296K
 - (R') Estimated accuracy on the temperature dependence coefficient n of the air pressure shift
- Water specific***
- (N') Estimated accuracy on the self broadened (HWHM) ($\text{cm}^{-1}\text{atm}^{-1}$) @296K
 - (S) Temperature dependence coefficient n of the self broadening halfwidth
 - (S') Estimated accuracy on the temperature dependence coefficient n of the self broadening HW
 - (T) Self pressure shift of the line transition ($\text{cm}^{-1}\text{atm}^{-1}$) @296K
 - (T') Estimated accuracy on the self pressure shift of the line transition ($\text{cm}^{-1}\text{atm}^{-1}$) @296K
 - (U) Temperature dependence coefficient n of the self pressure shift
 - (U') Estimated accuracy on the temperature dependence coefficient n of the self pressure shift

Standardized parameter missing values for GEISA-08 as a whole



FROM GEISA-03 TO GEISA-08: updated molecular species

MOI. ID	GEISA-03	SPECTRAL RANGE/ BAND ID.
	GEISA-03	GEISA-08 update
H ₂ O	0.007- 25232.004 cm ⁻¹	500- 8000 cm ⁻¹
CO ₂	436.123- 9648.007 cm ⁻¹	2200-7000 cm ⁻¹ 4000-9000 cm ⁻¹
O ₃	0.026- 4060.783 cm ⁻¹	1613- 4845 cm ⁻¹ 6000- 7000 cm ⁻¹
N ₂ O	0.838- 5131.249 cm ⁻¹	525- 10175 cm ⁻¹
CH ₄	0.010- 9199.285 cm ⁻¹	750- 1350 cm ⁻¹ 2850- 3150 cm ⁻¹ 4800- 9200 cm ⁻¹
O ₂	0.000- 15927.806 cm ⁻¹	0.7 μm region
SO ₂	0.017- 4092.948 cm ⁻¹	1011- 1410 cm ⁻¹
NO ₂	0.498- 3074.366 cm ⁻¹	780- 2940 cm ⁻¹
PH ₃	17.805- 2478.765 cm ⁻¹	770-3601 cm ⁻¹
HNO ₃	0.035- 1769.982 cm ⁻¹	Sub-millimeter U ₅ -U ₉ 2U ₉ -U ₉ U ₅ ; 2U ₉ (U ₈ +U ₉) ; (U ₆ +U ₇)



FROM GEISA-03 TO GEISA-08: updated molecular species (following)

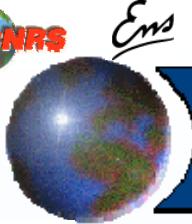
MOI. ID

SPECTRAL RANGE/ BAND ID.

GEISA-03

GEISA-08 update

H_2CO	0.000 - 2998.527 cm^{-1}	1.573 μm
C_2H_6	725.603 - 2977.926 cm^{-1}	12 μm region
CH_3D	7.760 - 3306.810 cm^{-1}	3250-3700 cm^{-1}
C_2H_2	604.774 - 3374.223 cm^{-1}	2.5 μm and 3.8 μm 1.5 μm region 0.83 μm region
C_2H_4	701.203 - 3242.172 cm^{-1}	1380- 1509 cm^{-1}
HCN	2.870 - 18407.973 cm^{-1}	14 μm (U_2 ; $2\text{U}_2-\text{U}_2$)
C_2N_2	203.955 - 2181.690 cm^{-1}	203.872 - 266.320 cm^{-1}
C_4H_2	190.588 - 654.425 cm^{-1} 605.5 - 651.4 cm^{-1}	199.1 - 244.0 cm^{-1}
HC_3N	474.293 - 690.860 cm^{-1} 20 μm (U_6)	16 μm (U_5)
HOCl	0.024 - 3799.249 cm^{-1}	3- 309 cm^{-1}
N_2	1992.628 - 2625.497 cm^{-1}	4.3 μm
CH_3Cl	674.143 - 3161.830 cm^{-1}	650 - 2650 cm^{-1}
H_2O_2	0.043 - 1499.487 cm^{-1}	0.043 - 1730 cm^{-1}



FROM GEISA-03 TO GEISA-08: updated molecular species (following)

MOI. ID

SPECTRAL RANGE/ BAND ID.

GEISA-03

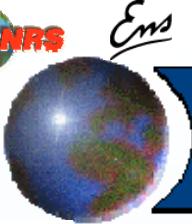
GEISA-08 update

HCOOH 1060.962 - 1161.251 cm⁻¹10 - 100 cm⁻¹940 - 1244 cm⁻¹SF₆ 940.425 - 952.238 cm⁻¹U₃, U₄, U_{4+U₆-U₆}C₃H₄ 290.274 - 359.995 cm⁻¹290 - 360 cm⁻¹592 - 673 cm⁻¹ClONO₂ 763.641 - 790.805 cm⁻¹500 - 1330 cm⁻¹

27 molecular species
updated

6 New Molecular Species

CH₃Br 16 μmCH₃OH 0.02 - 33 cm⁻¹
10 μm regionNO+ 1635- 2530 cm⁻¹HNC 0.22 - 12594 cm⁻¹C₆H₆ 642 - 705 cm⁻¹C₂HD 451 - 580 cm⁻¹
600 - 760 cm⁻¹



FROM GEISA-03 TO GEISA-08: non-updated molecular species

MOI.

GEISA-03

MOI.	GEISA-03
CO	3.414 - 8464.882 cm ⁻¹
NO	0.000 - 9273.214 cm ⁻¹
NH ₃	0.058 - 5294.502 cm ⁻¹
OH	.005 - 35877.031 cm ⁻¹
HF	41.111 - 11535.570 cm ⁻¹
HCl	20.240 - 13457.841 cm ⁻¹
HBr	16.232 - 9758.565 cm ⁻¹
HI	12.509 - 8487.305 cm ⁻¹
ClO	0.015 - 1207.639 cm ⁻¹
OCS	0.381 - 4118.004 cm ⁻¹
GeH ₄	937.371 - 2224.570 cm ⁻¹
C ₃ H ₈	700.015 - 799.930 cm ⁻¹
H ₂ S	2.985 - 4098.234 cm ⁻¹
COF ₂	725.006 - 2001.348 cm ⁻¹
HO ₂	0.173 - 3675.819 cm ⁻¹

Updates for 2008 Edition of GEISA/IASI line transition parameters sub-database

Preliminary non exhaustive list

Molecular species already archived in GEISA/IASI

H ₂ O	500- 8000 cm ⁻¹	LISA, JPL
CO ₂	2200-7000 cm ⁻¹	JPL, LTS
N ₂ O	1900-6800 cm ⁻¹	JPL
CH ₄	750-1350 cm ⁻¹	ICB, JPL
	2850-3150 cm ⁻¹	
SO ₂	U ₁ , U ₃	LISA
	U ₁ +U ₂ -U ₂	GSMA
HNO ₃	U ₅ ; 2U ₉	LISA
C ₂ H ₂	604- 2254 cm ⁻¹	LADIR

Molecular species related with IASI Trace Gas Retrievals to be added

HCN
NH₃
HCOOH
C₂H₄
CH₃OH

New PF 3.2 Version (courtesy of J.M. Flaud) to be considered

7 molecular species updated

GEISA-08 line transition parameters sub-database

2) Evaluation of the impact
of H₂O spectroscopic archive differences using IASI
4A/STRANSAC Radiative transfer
simulations

4A (Automatized Atmospheric Absorption Atlas);
fast and accurate line-by-line radiative transfer model
[N.A. Scott and A. Chédin, 1981; Tournier et al. 1995; Chéruy et al. 1995]

 **STRANSAC** [N.A. Scott, 1974]
line-by-line and layer-by-layer model

in their **latest 2000 version**

Selected Spectroscopic Databases

Differences in contents and subsequent IASI radiative transfer modelling

GEISA/IASI-03

Jacquinet-Husson N. et al. *JQSRT* 95 (2005) 429-467.

GEISA/IASI-08 update with:

- Toth R.A. « Linelist of water vapor parameters from 500-8000 cm⁻¹ » *JQSRT (in preparation)*.
<http://mark4sun.jpl.nasa.gov>
- Coudert L. H. et al. « The eight first vibrational states of the water molecule: measurements and analysis» *J.M.S.* 228, 471-498 (2004); « The water molecule: line position and line intensity analyses up to the second triad » *J.M.S., in preparation*.

Spectral intervals: 600-800 cm⁻¹ 1300-1500 cm⁻¹ 1700-2000 cm⁻¹

MIPAS Dedicated Spectroscopic Database Version PF 3.2

Flaud et al. *J. Atm. And Ocean Optics*, 16 (2003) 172-182.

HITRAN-04

Rothman et al. *JQSRT* 96 (2005) 139-204.

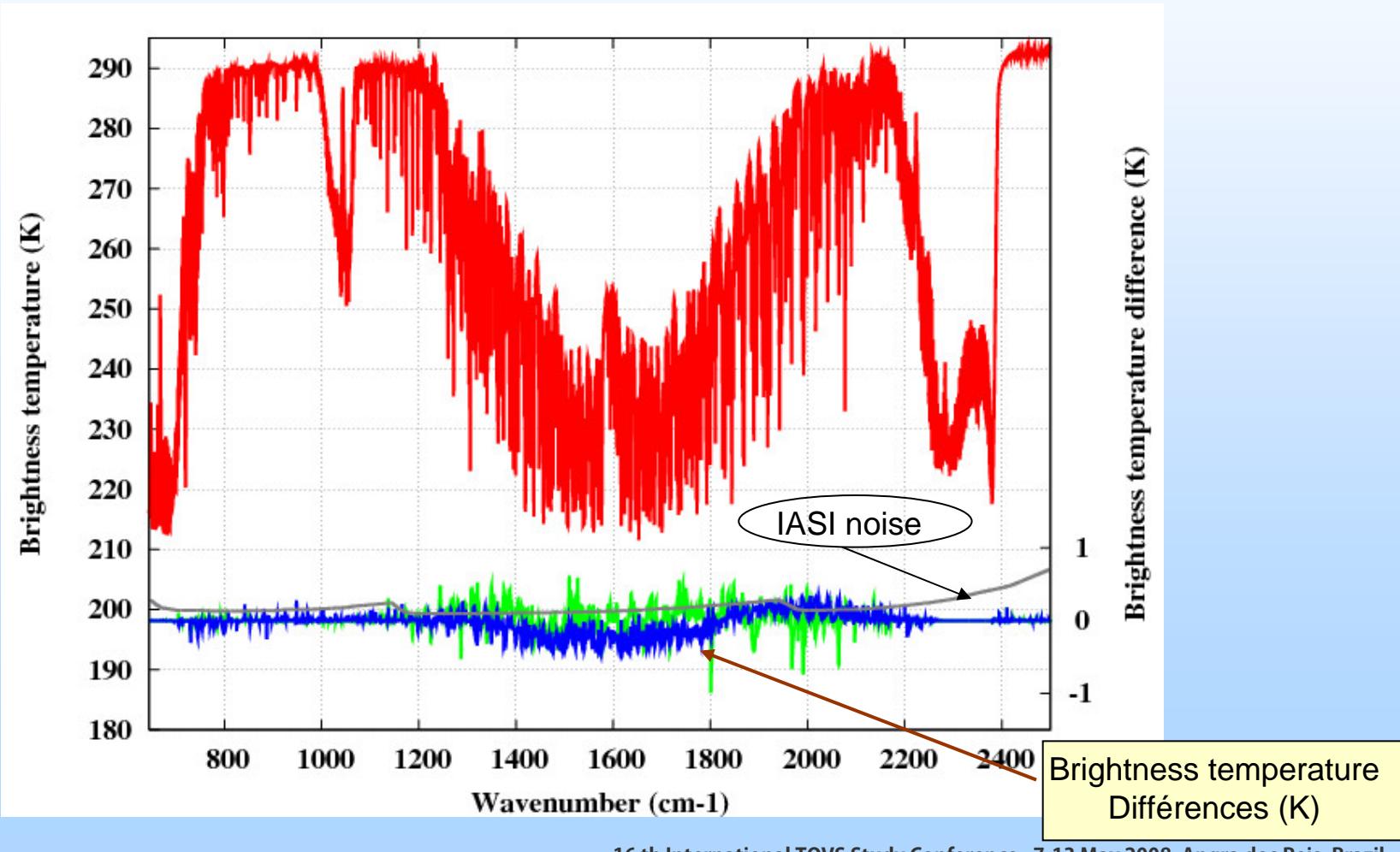
HITRAN-06 update with:

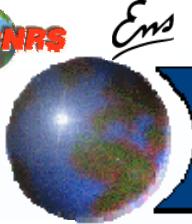
Gordon et al. "Current updates of the water-vapor line list in HITRAN: a new "diet" for air-broadened half-width". *JQSRT* 108 (2007) 389-402.



H₂O Spectroscopy differences illustration

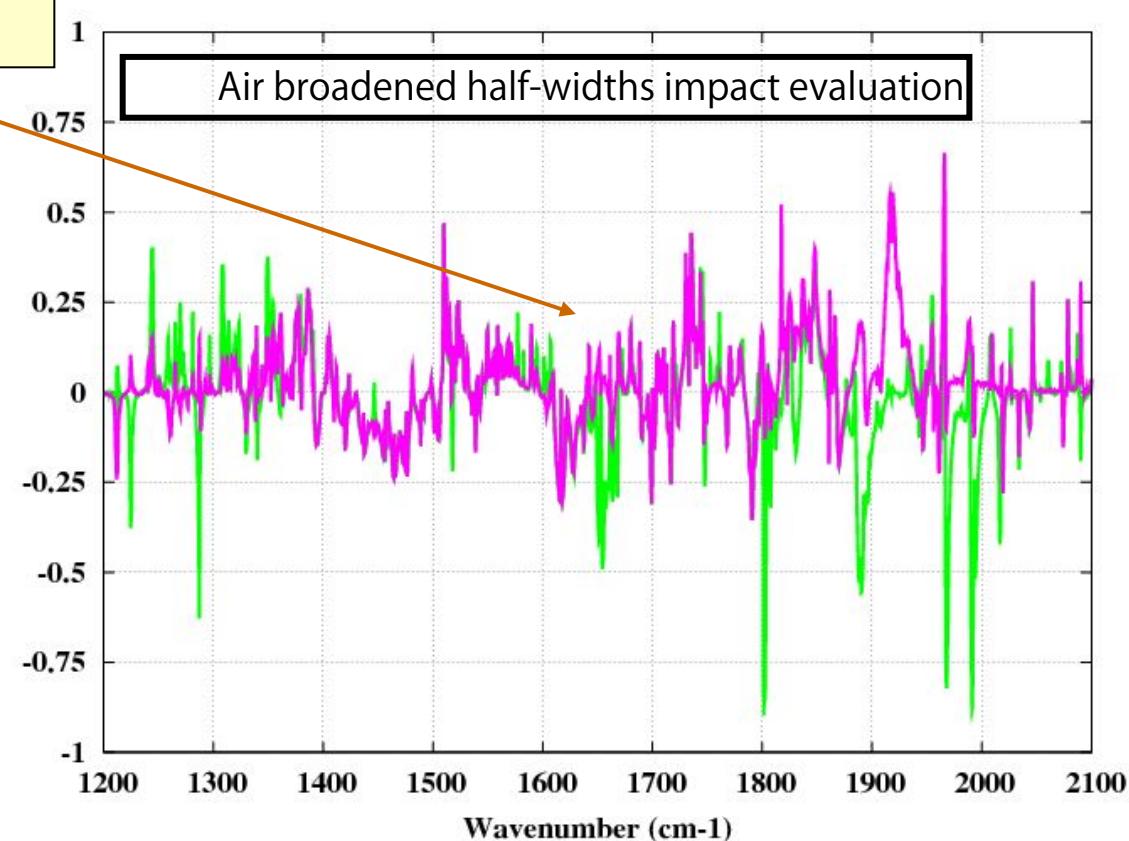
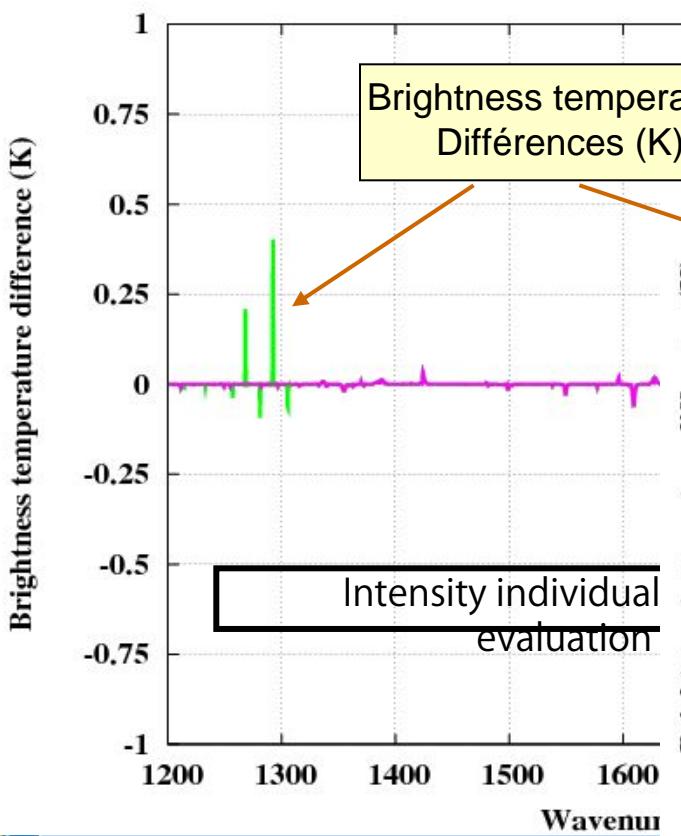
- ❖IASI brightness temperature (K) simulation with **GEISA-03** (upper curve);
- ❖Impact of replacement of **HITRAN-04** or **MIPAS PF3.2 H₂O data** in GEISAIASI-03
- ❖differences (K) in lower curves, with associated **IASI noise**.





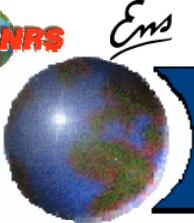
Individual impact of Spectroscopic parameters

GEISA-03 IASI brightness temperature simulation differences (K), replacing H₂O spectroscopy by HITRAN-04 or HITRAN-06 one



GEISA-08 line transition parameters sub-database

3) Evaluation of the impact
of H₂O spectroscopic archive differences using
**IASI Metop Flight Data and 4A/STRANSAC Radiative
transfer simulations**

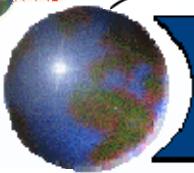


Evaluation Process

- + From the IASI level1b data (from Ether server), a set of 69 IASI spectrums have been selected for the period of August 2007 to February 2008.
- + A collocation with the ECMWF radiosoundings have been made with a colocation's distance of : space = 100 km; time = less than 1 hour.
- + This dataset has been used to identify the quality of the update of GEISA-2008, in comparison with GEISA-2003 and HITRAN-2006 H₂O archives.
- + Two specific spectral regions have been selected:
 $800\text{-}900\text{ cm}^{-1}$ and $1800\text{-}2000\text{ cm}^{-1}$.
- + Whereas the first region don't show improvement in the spectroscopic parameters, the second seems to show a comparaison closest to the IASI observations with GEISA-2008.

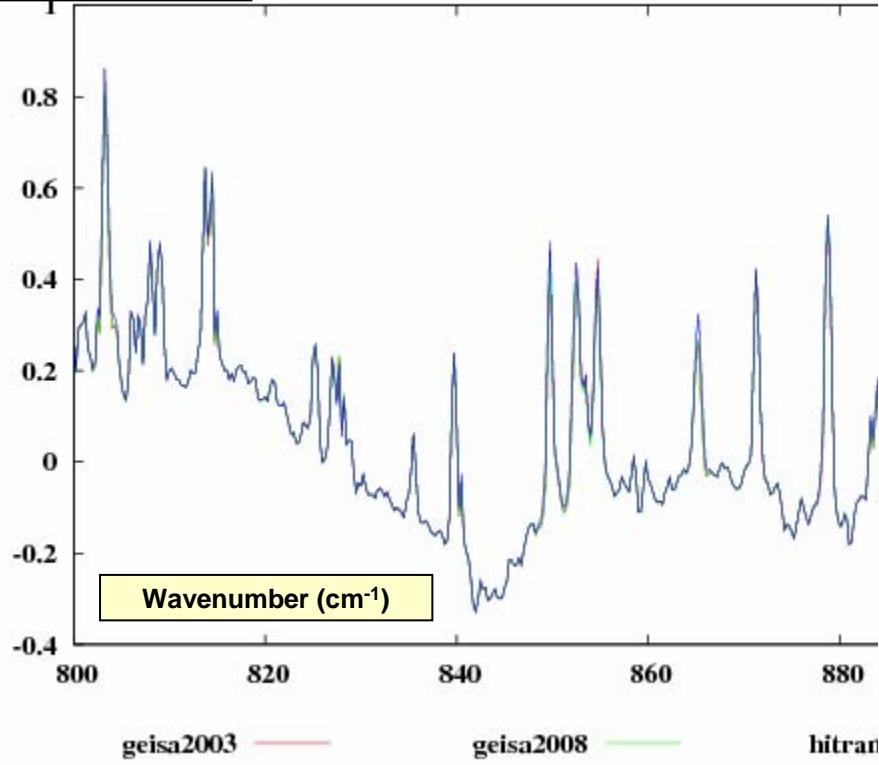
These preliminary results have to be confirmed.

Especially, the quality of the spectra have to be examined, and the number of collocations has to be increased.

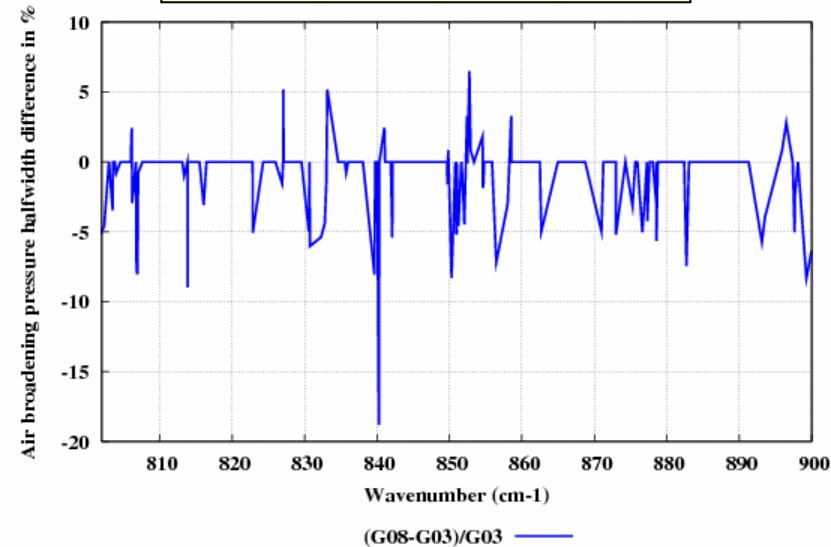


800 – 900 cm⁻¹ IASI Observations

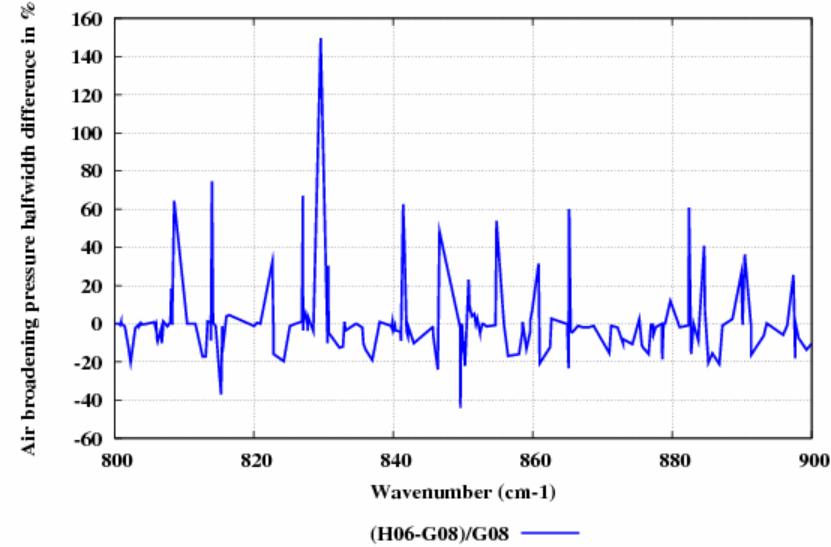
Brightness temperature
différences (K)

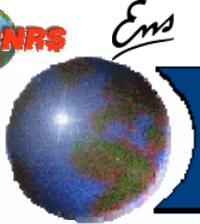


GEISA-03 vs GEISA-08
Air-broadening HW differences (%)

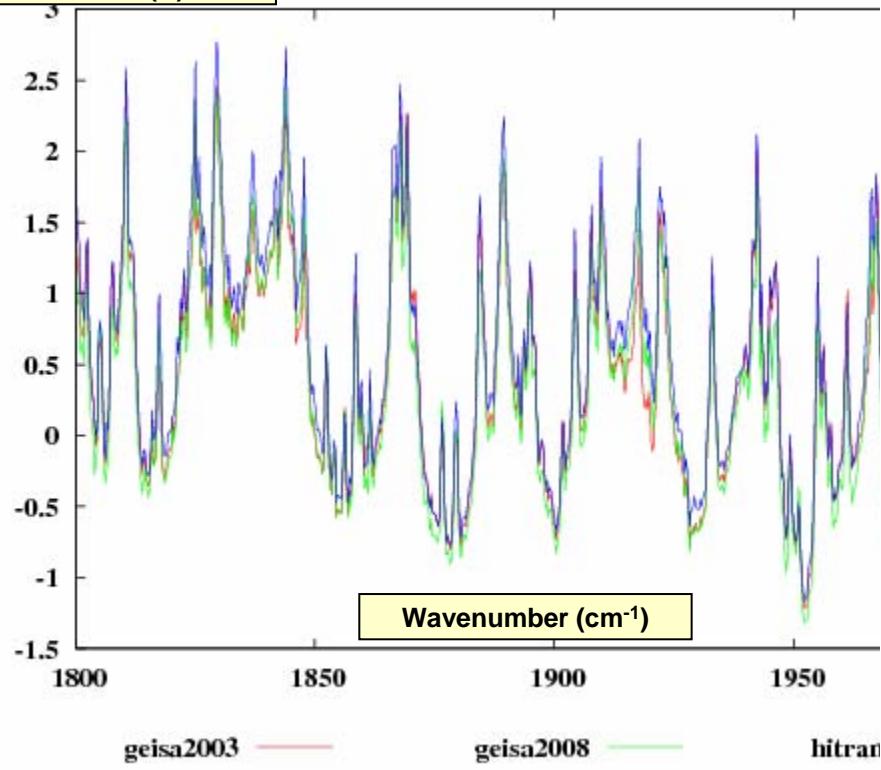


GEISA-03 vs HITRAN-06
Air-broadening HW differences (%)



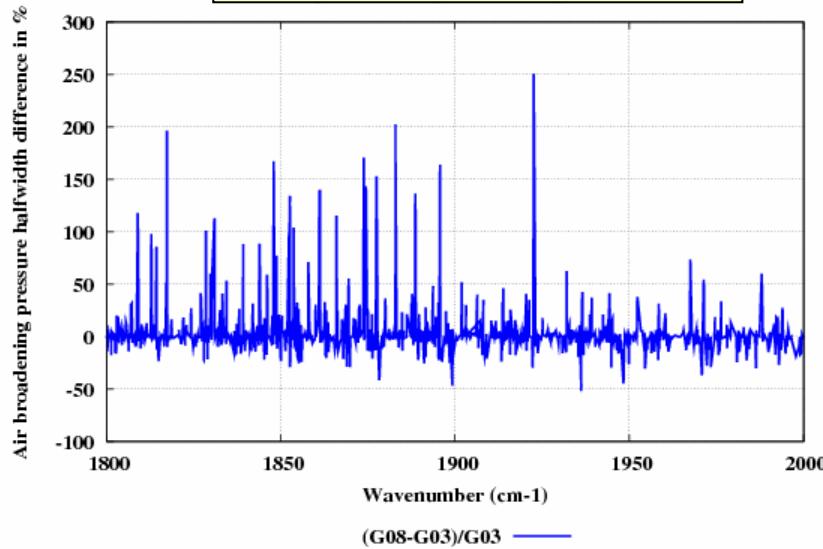


**Brightness temperature
Différences (K)**

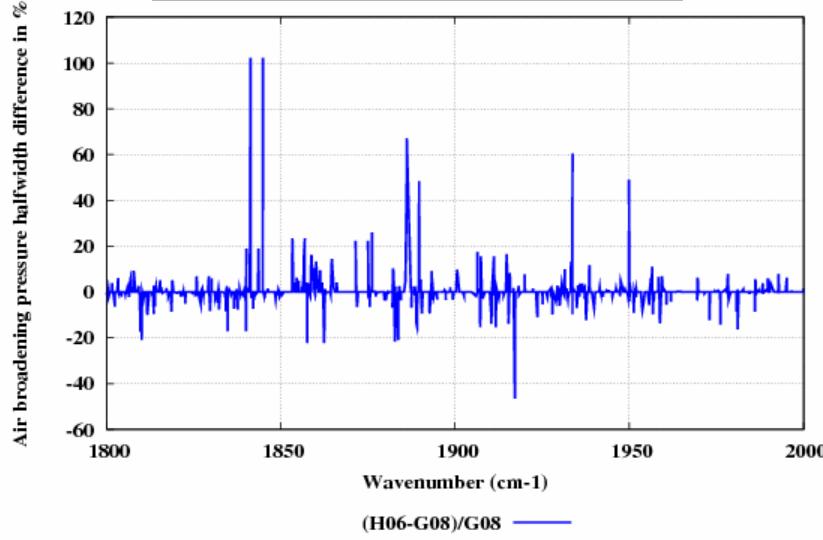


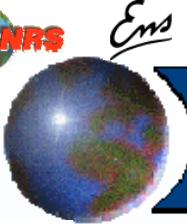
1800 – 2000 cm^{-1} IASI Observations

**GEISA-03 vs GEISA-08
Air-broadening HW differences (%)**



**GEISA-03 vs HITRAN-06
Air-broadening HW differences (%)**

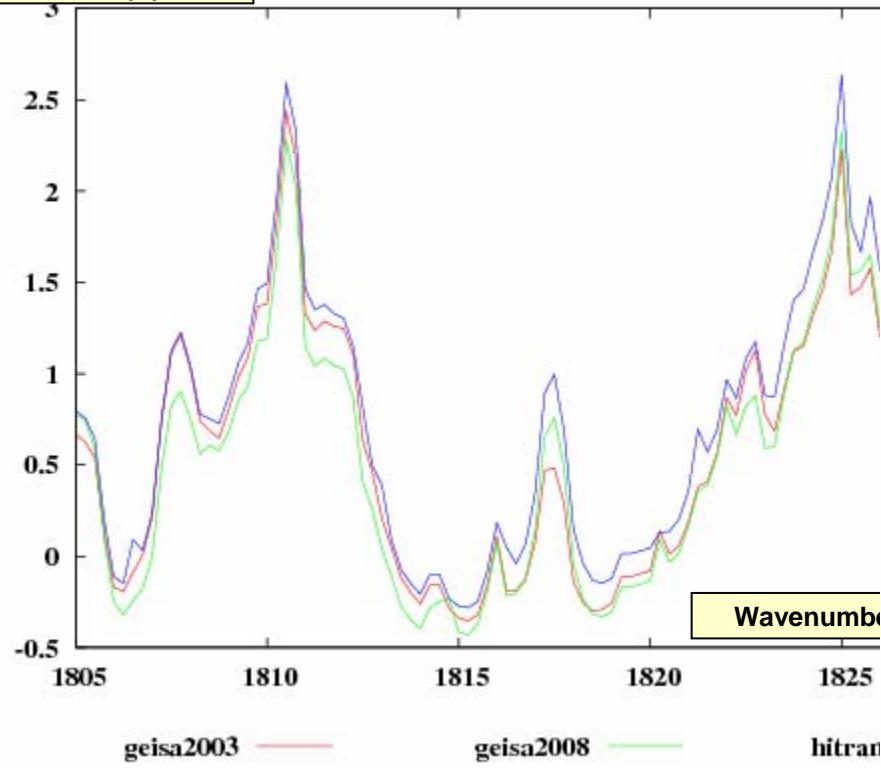




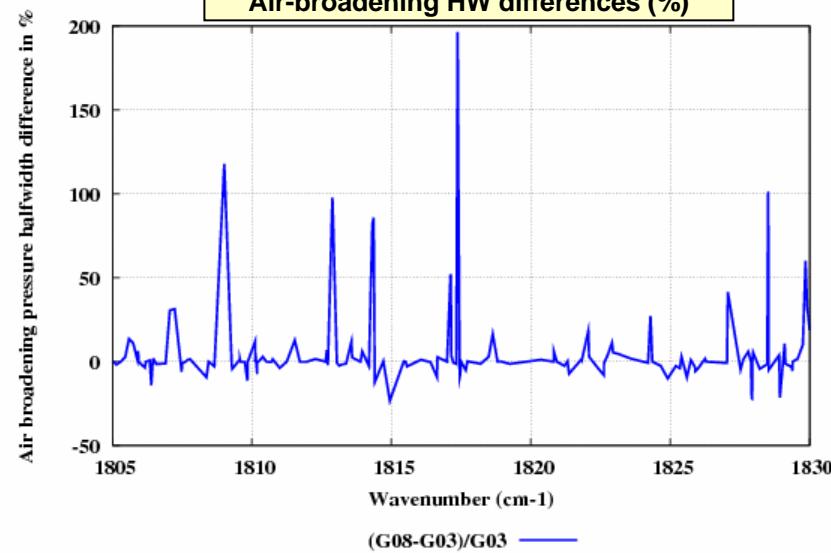
ZOOM 1805 – 1830 cm^{-1} IASI Observations

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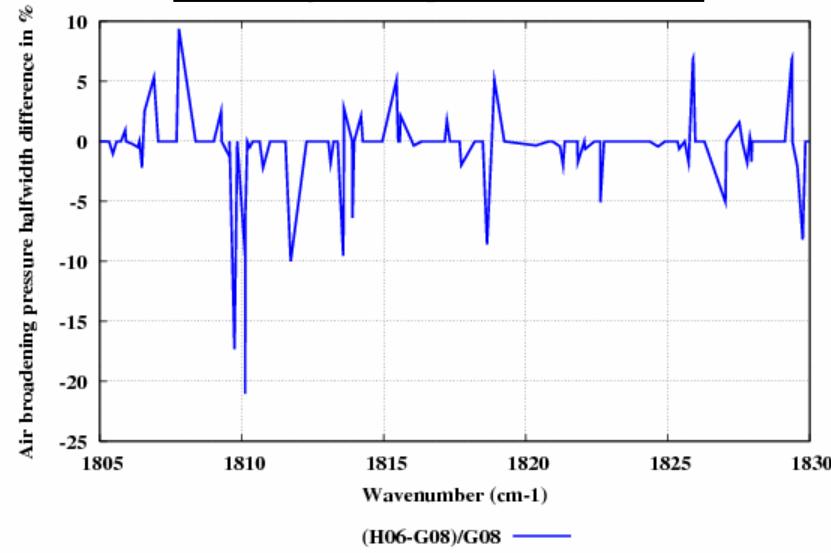
Brightness temperature
différences (K)



GEISA-03 vs GEISA-08
Air-broadening HW differences (%)



GEISA-03 vs HITRAN-06
Air-broadening HW differences (%)





Concluding Comments





Remaining spectroscopy related problems

Some conclusions of validation exercises, using e.g. : the 4A-00/LMD Model, in the case of IASI radiative transfer modelling

1. **The water vapour spectroscopic parameters:** still need to be validated;
2. **The water vapour continuum:** more tuning to be done when more validation data (especially with high water vapor content) become available;
3. **The freons bands at 850 and 920 cm⁻¹:** refine the temperature dependence;
4. **O₃ in the 9.6 μm region:** the spectroscopic parameters still need to be validated;
5. **Some CO₂ – Q branches:** further improvement/tuning of the line mixing (15 μm region especially)

Forward Models Error Sources

Spectroscopy and RT model

- line inaccurate positions, line intensities, halfwidths, ...
- unsufficient/missing information (absorbers, hot bands, heavy molecules cross sections, ...)
- line shape, continua, line coupling,...
- pressure shift
- NLTE

*Courtesy A. Chédin, Trattoria/CNES
2-3 April 2008*

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THANK YOU FOR YOUR ATTENTION