How it could be possible to evaluate the spectroscopic parameters: the example of the new release of GEISA-2019

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Requirements from the spatial agencies :

- What is the precision of the spectroscopy ?
- What could be the part of the spectroscopy on the global budget error of a given mission ?
- Is it sufficient according to a given mission requirement ?

The method

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LMD

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Evaluation of spectroscopic databases through radiative transfer simulations compared to observations. Application to the validation of GEISA 2015 with IASI and TCCON

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ABSTRACT

The quality of spectroscopic parameters that serve as input to forward radiative transfer models are essential to fully exploit remote sensing of Earth atmosphere. However, the process of updating spectroscopic databases in order to provide the users with a database that insures an optimal characterization of spectral properties of molecular absorption for radiative transfer modeling is challenging. The evaluation of the databases content and the underlying choices made by the managing team is thus a crucial step. Here, we introduce an original and powerful approach for evaluating spectroscopic parameters: the Spectroscopic Parameters And Radiative Transfer Evaluation (SPARTE) chain. The SPARTE chain relies on the comparison between forward radiative transfer simulations made by the 4A radiative transfer model and observations of spectra made from various observations collocated over several thousands of well-characterized atmospheric situations. Averaging the resulting 'calculated-observed spectral' residuals minimizes the random errors coming from both the radiometric noise of the instruments and the imperfect description of the atmospheric state. The SPARTE chain can be used to evaluate any spectroscopic databases, from the visible to the microwave, using any type of remote sensing observations (ground-based, airborne or space-borne). We show that the comparison of the shape of the residuals enables: (i) identifying incorrect line parameters (line position, intensity, width, pressure shift, etc.), even for molecules for which interferences between the lines have to be taken into account; (ii) proposing revised values, in cooperation with contributing teams; and (iii) validating the final updated parameters. In particular, we show that the simultaneous availability of two databases such as GEISA and HITRAN

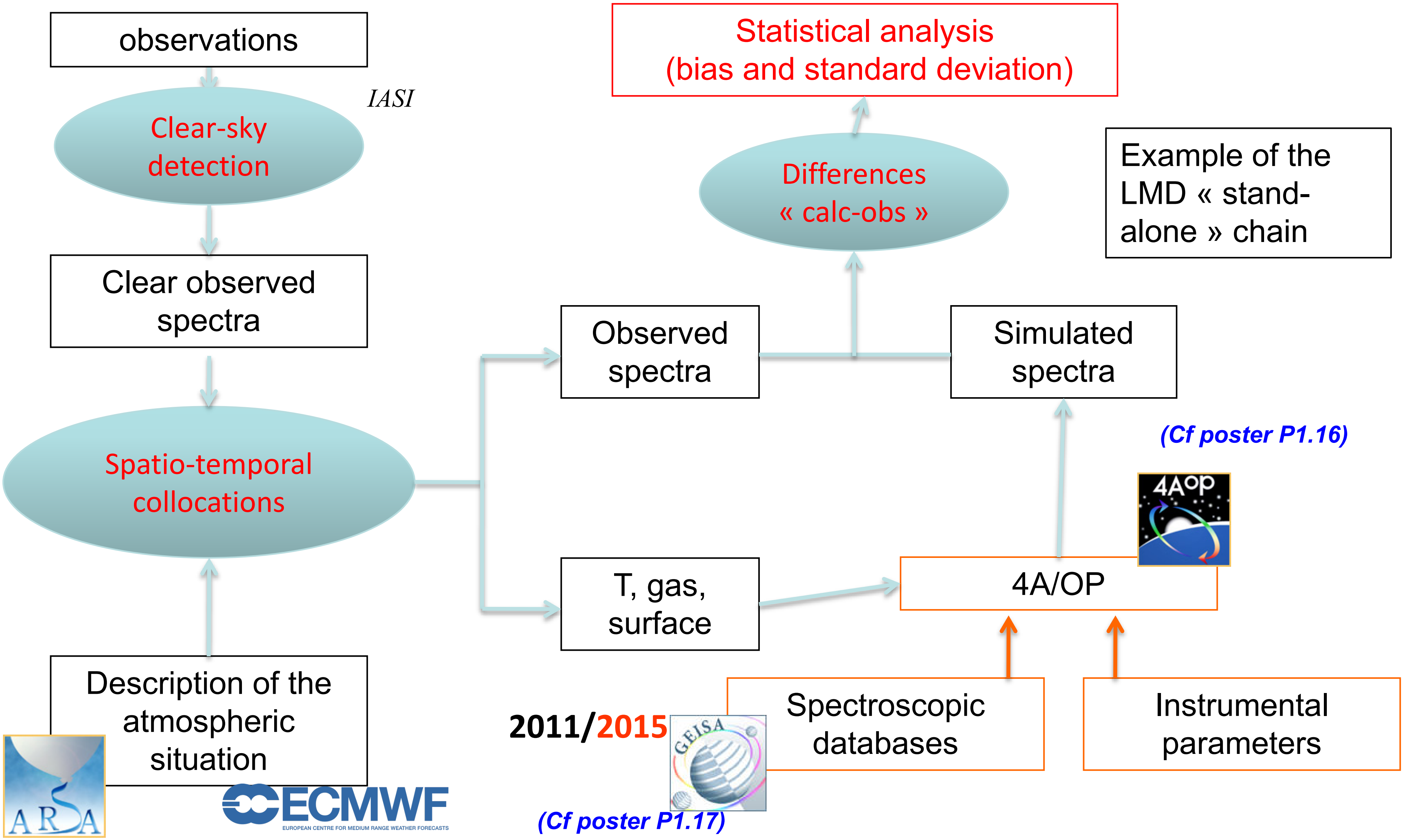
In the frame of the GEISA 2015 update, development of a quasi automatic chain to evaluate the spectroscopic parameters received from a laboratory

➔ Feedbacks to the laboratory before the finalization of the GEISA database

The method

SPARTE: Spectroscopic Parameters And Radiative Transfer Evaluation

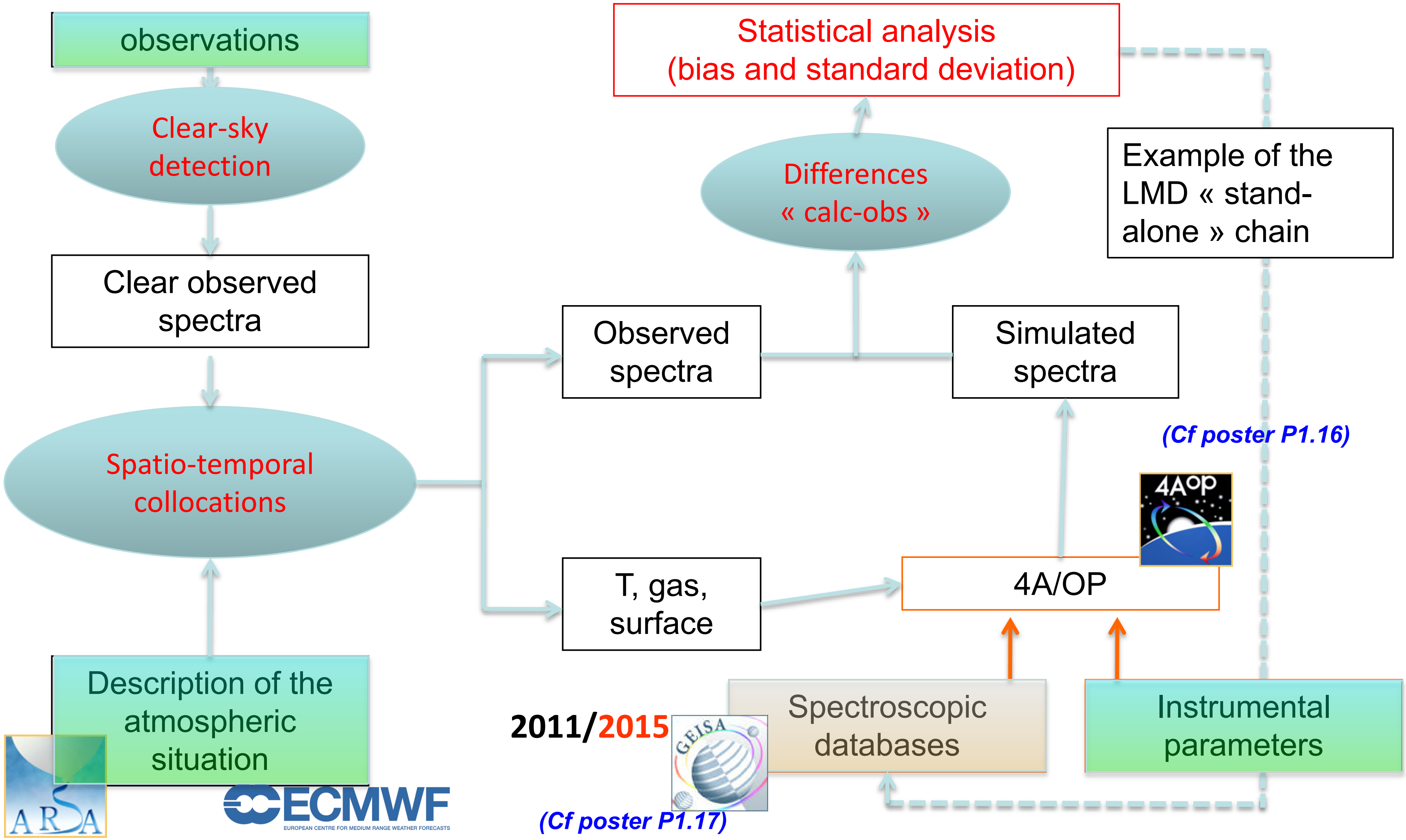
Armante et al, JMS, 2016, vol 327



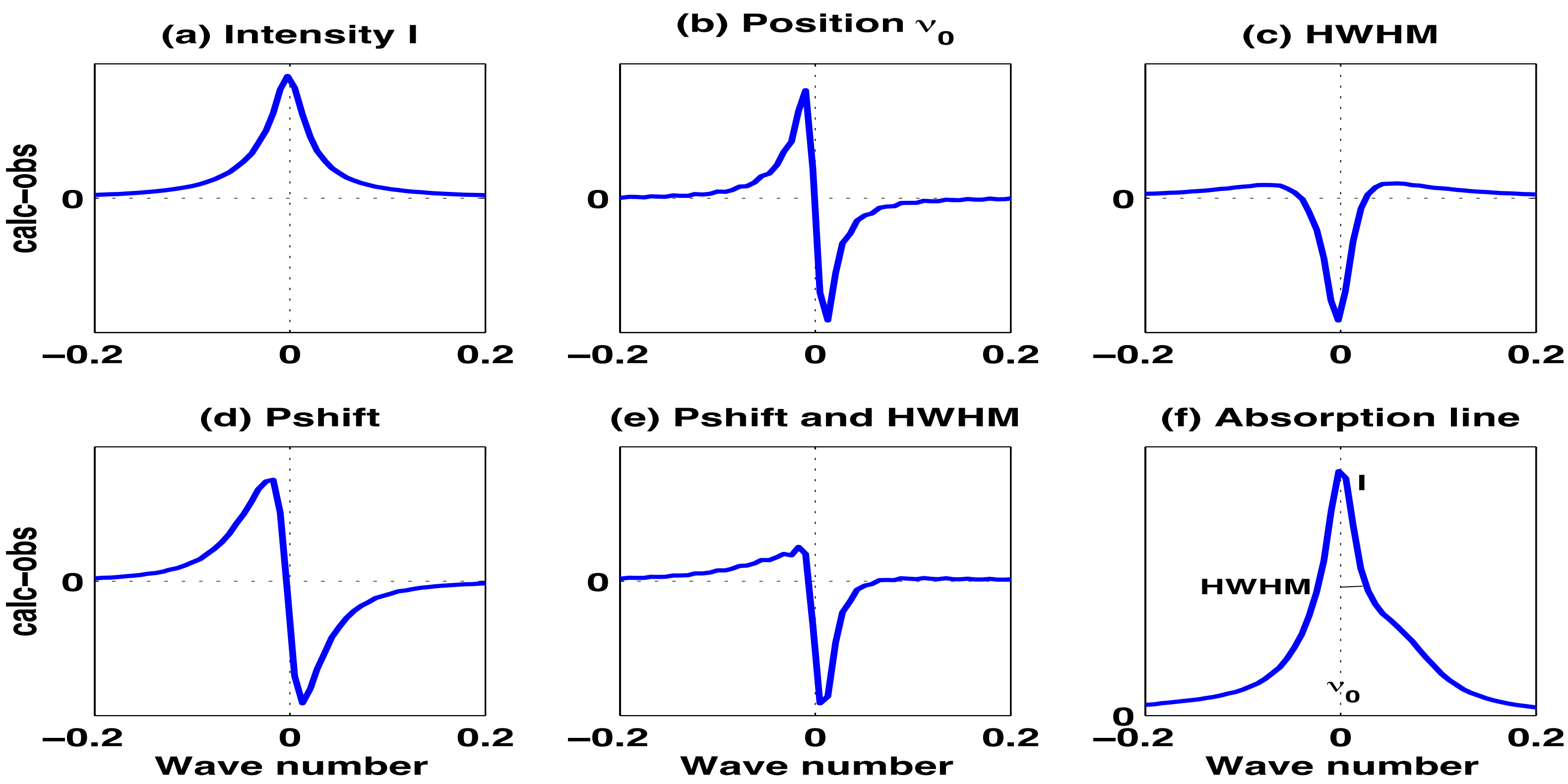
The method

SPARTE: Spectroscopic Parameters And Radiative Transfer Evaluation

Armante et al, JMS, 2016, vol 327



With well-resolved instruments, the shape of the residual can indicate which spectroscopic parameter is involved



Cf Armante et al, 2016, JMS

The method

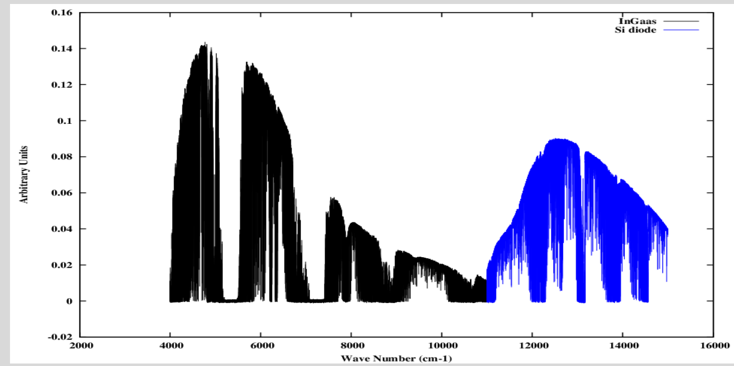
NIR

Ground-based data - TCCON network

Fourier transform spectrometer (HR/FTS)

- 2 detectors:
  - Ingaas (4000-11000 cm^{-1})
  - Si-diode (11000-14000 cm^{-1})

Spectral resolution : $7.3x10^{-3}$ cm^{-1}



https://tccon-wiki.caltech.edu/

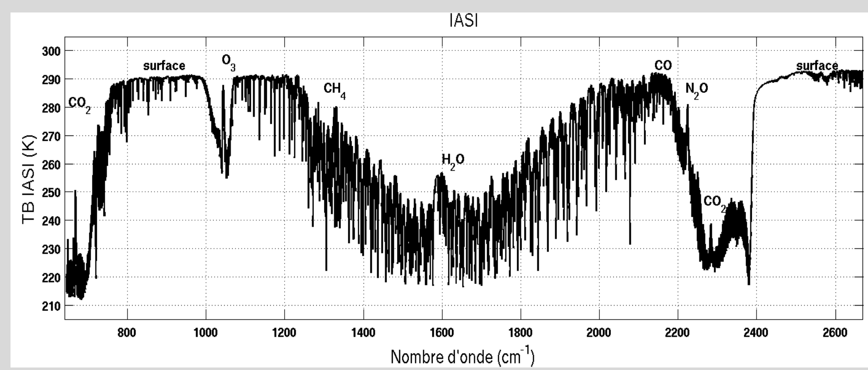
➔ 2760-4000 cm-1 with ACE-FTS instrument in progress …

TIR

The IASI instrument

IASI characteristics :

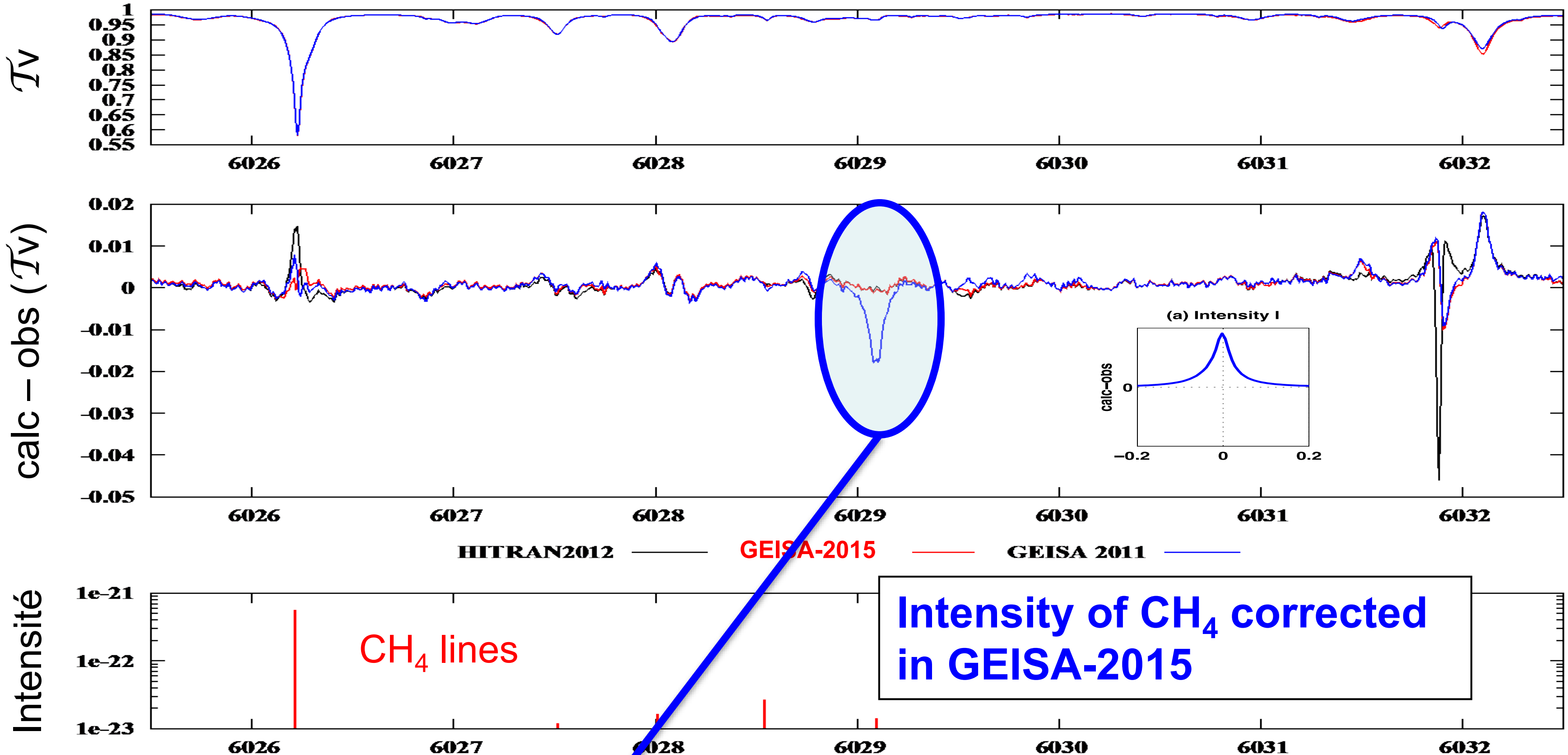
- 8461 spectral channels between 645 and 2760 cm^{-1} (15.5 - 3.63 µm)
- spectral resolution of 0.5 cm^{-1} after apodisation (“Level 1c” spectra)
- spectral sampling interval is 0.25 cm^{-1}
- nadir FOV: 12 km



IASI instrumental noise ~ 0.25 K

The method

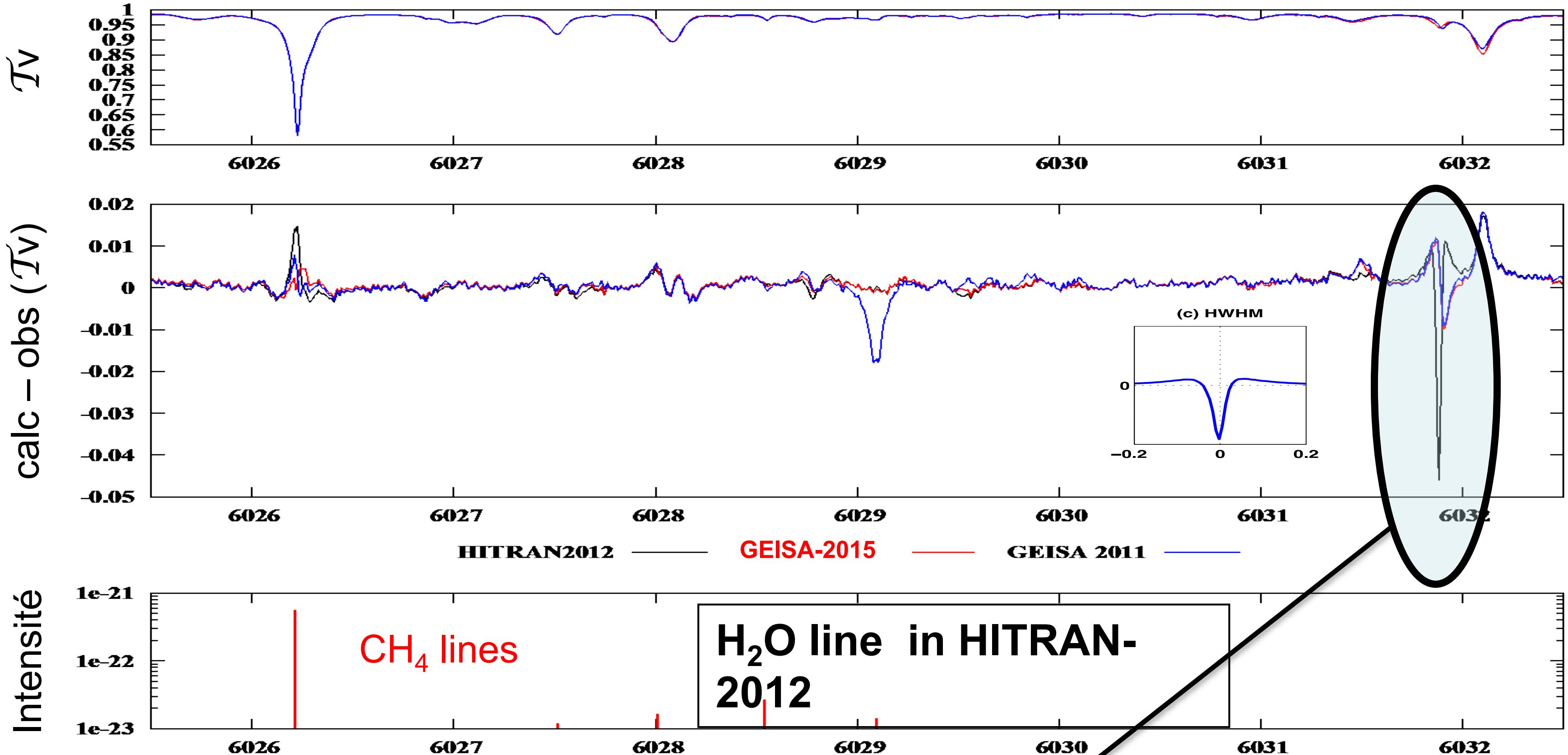
Evaluation of CH_4 and H_2O in GEISA-2015 for the 1.65 µm band



	Position	Intensity	HWHM	E0	n				P shift
GEISA-2011	6029.082800	1.1090D-23	0.0655	62.8798	0.85	311	6	L08	-0.011060
GEISA-2015	6029.107870	1.4250D-23	0.0600	62.9000	0.85	311	6	AC3	-0.012058
HITRAN-2012	6029.107870	1.4250D-23	0.0657	62.8811	0.73	311	6	H12	-0.012100

The method

Validation of CH_4 and H_2O in GEISA-2015 for the 1.65 µm band



	Position	Intensity	HWHM	E0	n				P shift
GEISA-2011	6031.899390	7.3020D-26	0.0300	2042.31	0.36	161	1	T03	-0.000000
GEISA-2015	6031.899400	7.1300D-26	0.0380	2042.31	0.41	161	1	L13	-0.011060
HITRAN-2012	6031.899390	7.3020D-26	0.0078	2042.31	0.36	161	1	H12	-0.022000

Validation of GEISA-2019 O3

Open issue: Discrepancies between the different spectral ranges (UV, TIR, …) in the intensities ➔ too many differences in the O3 retrievals

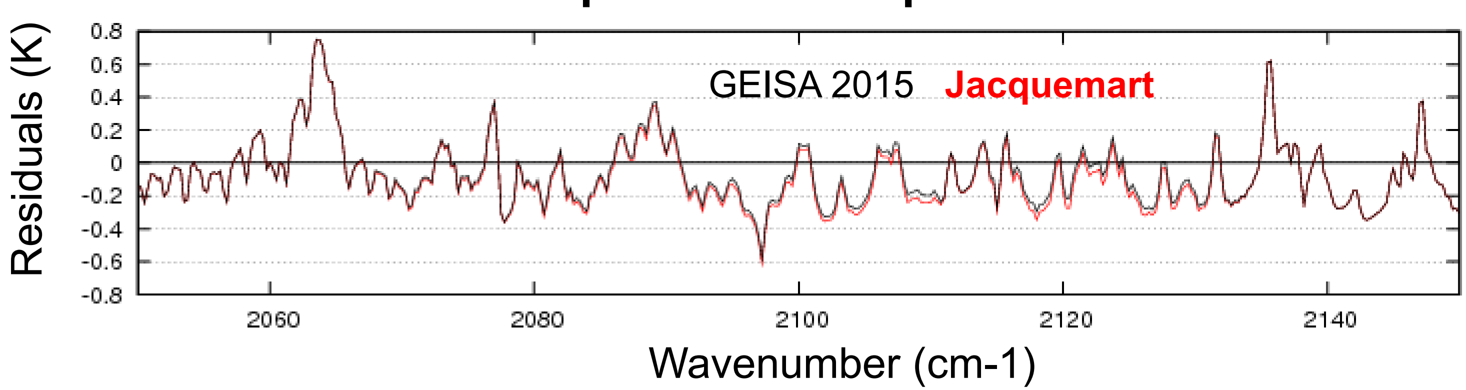
IASI and IASI-NG between the 9.6 and the 5 µm bands

➔ High effort to estimate the absolute intensity of O3 in each band

<u>GEISA 2019 Update</u>

Compilation done by the GSMA (Reims, Tyuterev) with work of different contributors : Barbe, Birk, Jacquemart/Janssen, Tyuterev, …

Minor update in the 5 µm band



Validation of GEISA-2019 O3

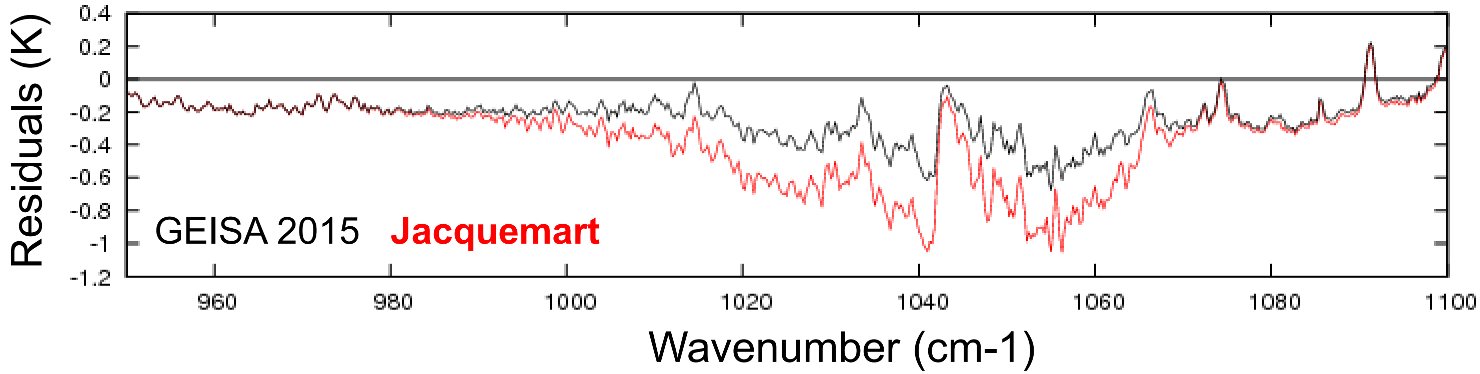
Open issue: Discrepancies between the different spectral ranges in the intensities ➔ too many differences in the O3 retrievals

Possible case for IASI and IASI-NG between the 9.6 and the 5 µm bands

➔ High effort to estimate the absolute intensity of O3

GEISA 2019 Update

Compilation done by the GSMA (Reims, Tyuterev) with work of different contributors : Barbe, Birk, Jacquemart/Janssen, Tyuterev, …



higher residual in the 9.6 µm band

Feedback to the laboratory has permitted to find a problem in the calibration of the measurements used to elaborate the line list ➔ new line list in progress …

Validation of GEISA-2019 CO_2

- **Perevalov (CDSD catalog based on measurements)**
- Zack (model, *ab initio*)

Evaluation more complicated due to the line mixing effects …

CO2 modelling …

➔Spectroscopic parameters G15 vs Perevalov

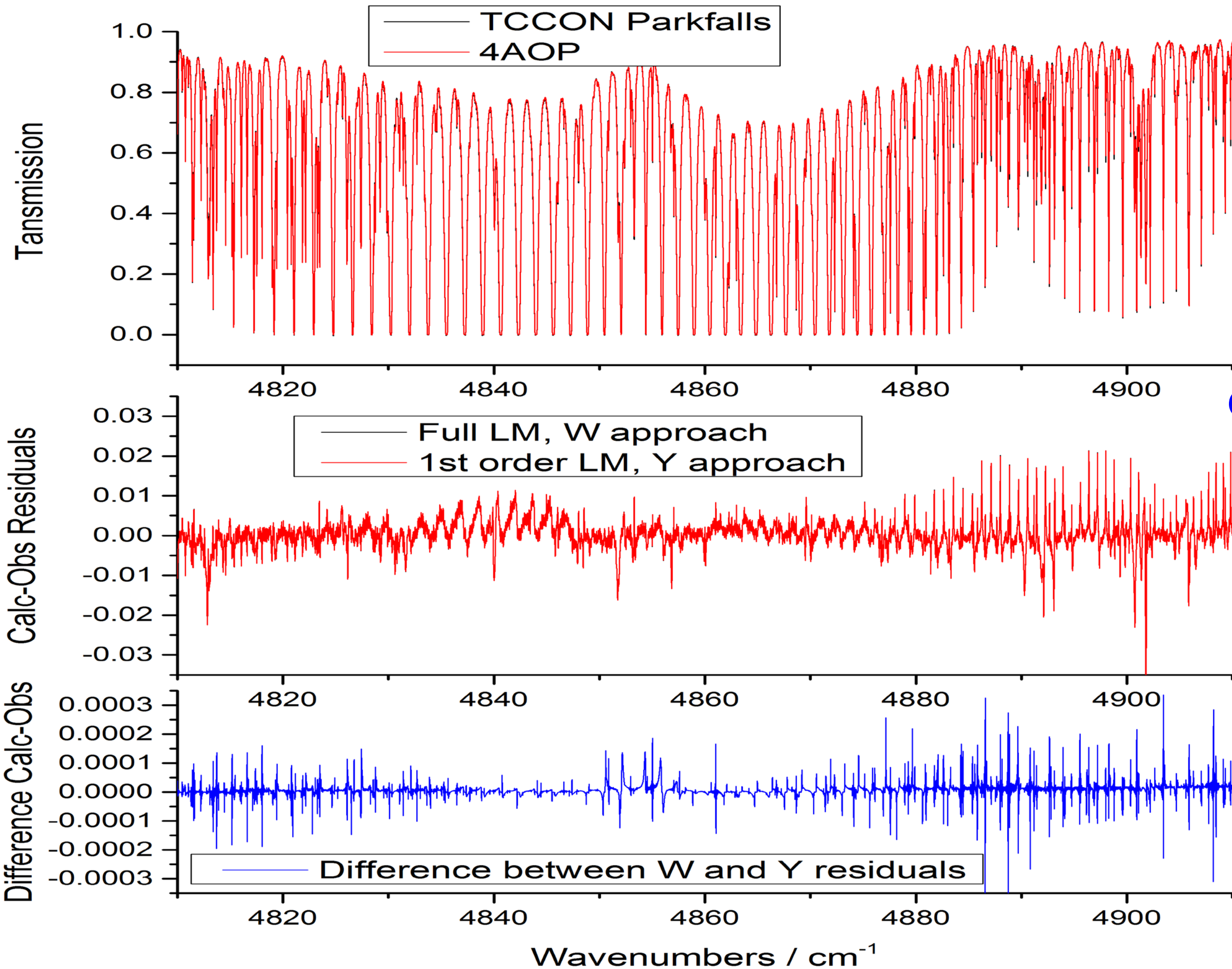
➔Wfull : Full matrix line mixing (Lamouroux 2012)
➔Y: First order line mixing
➔Y SD: First order line mixing + Speed dependent/ Dicke effects (Lamouroux 2015)

Tools from Lamouroux et al, 2015 available at LMD ➔ can study the impact of the spectroscopic parameters

Note: No Speed dependent Voigt profile can be used when the full relaxation matrix is used

Validation of GEISA-2019
CO2

CO2 modelling … Comparison Y vs Wfull ➔ Y is a good approximation in the SWIR

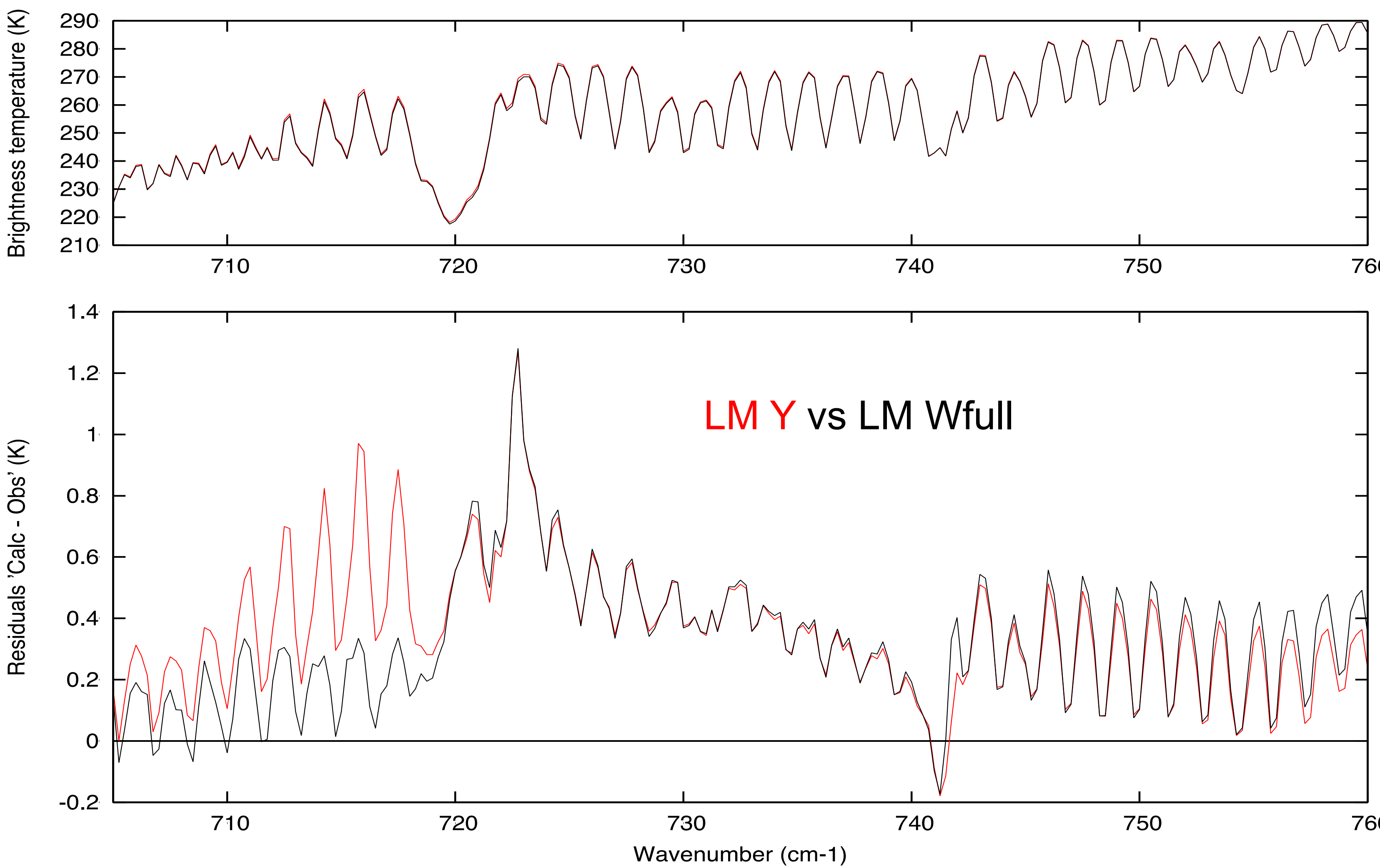


OCO-2 and Microcarb

Validation of GEISA-2019 CO_2

LMD

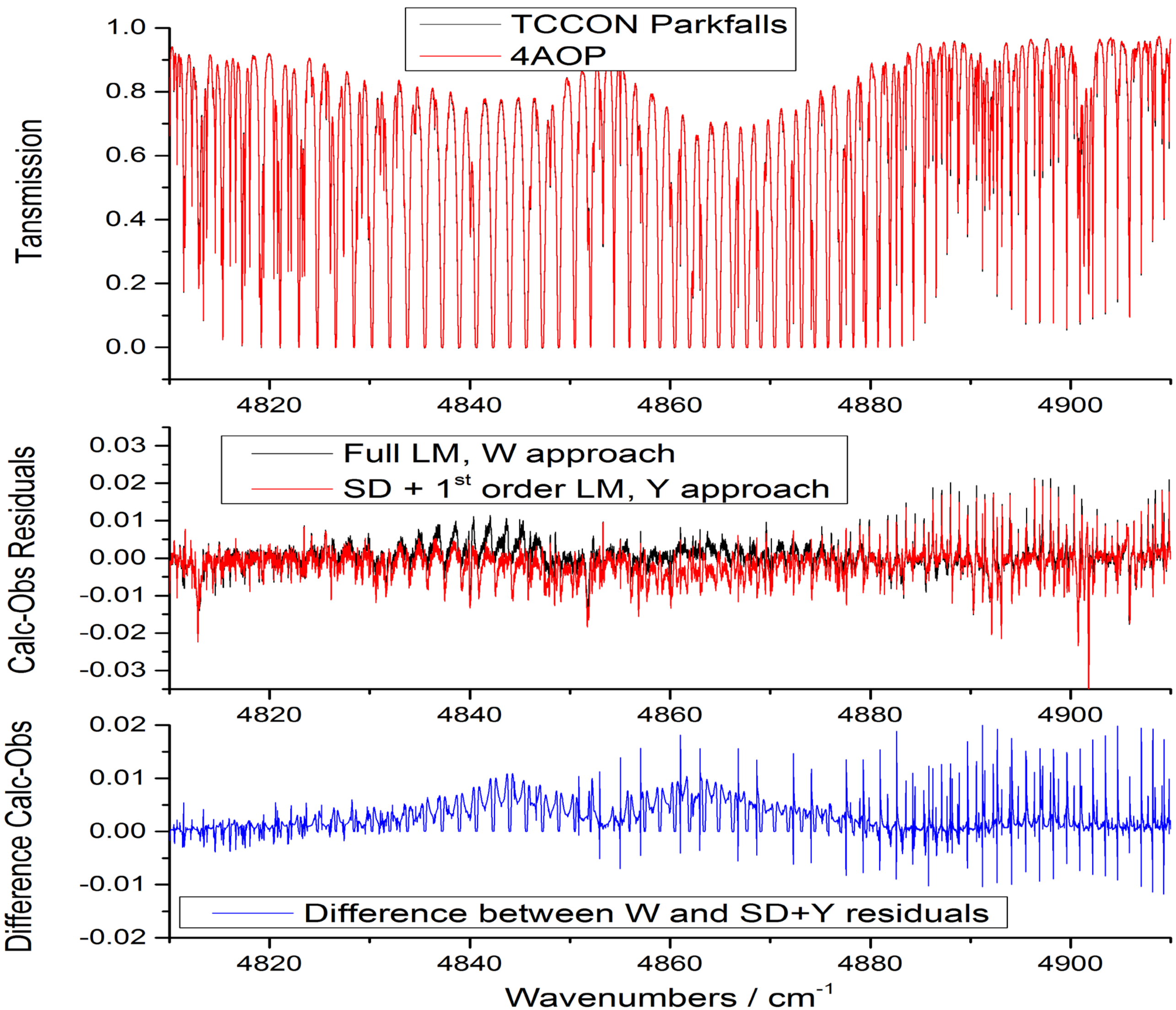
CO_2 modelling … Comparison Y vs Wfull ➔ too important error with the LM Y in the TIR



Validation of GEISA-2019 CO_2

LMD

CO_2 modelling … comparison SD vs Wfull ➔ important positive impact

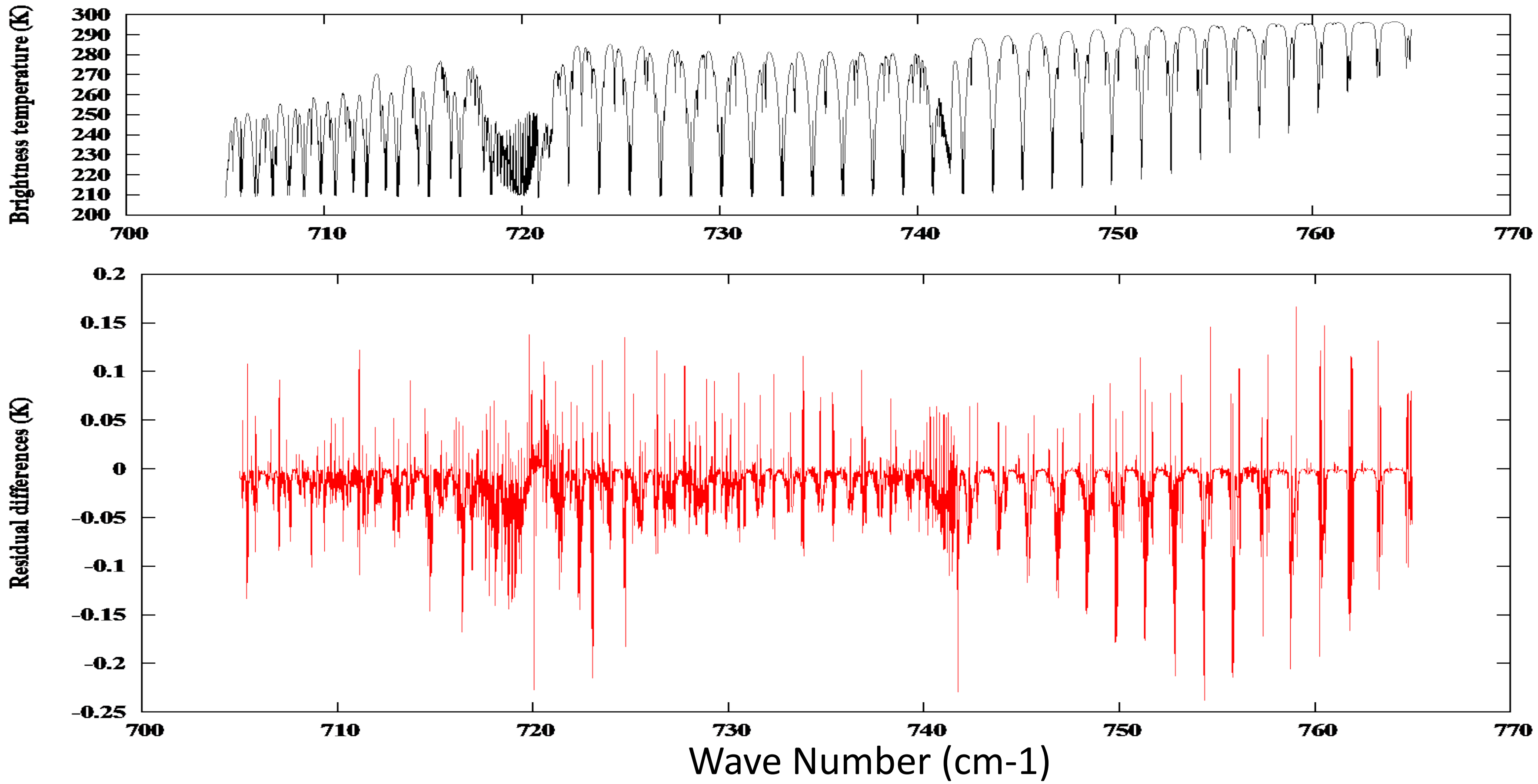


Strong impact for OCO-2 and Microcarb

Validation of GEISA-2019 CO2

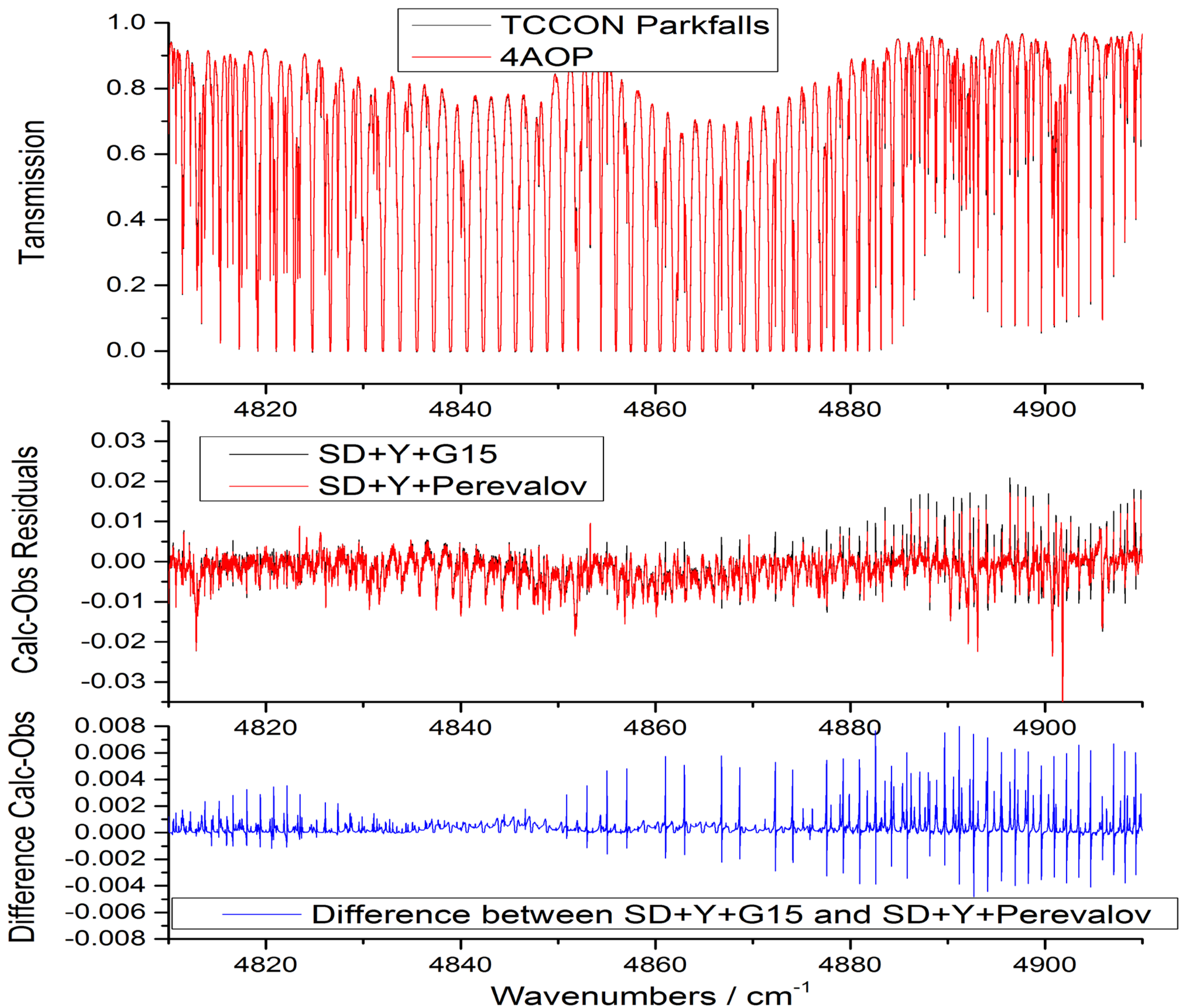
CO2 modelling … comparison Perevalov vs G15 ➔ weak impact

IASI simulation : LM GEISA-2015 vs LM Perevalov 2019



Validation of GEISA-2019 CO_2

CO2 modelling … Comparison Perevalov vs G15 → positive impact



→ Keep Perevalov in GEISA-2019

Validation of GEISA-2019 H_2O/HDO

GEISA 2019 Update

- Birk: H_2O (1850 → 4439 cm-1), HDO (2478 → 4439 cm-1) Speed Dependent (SD) line profile
- Coudert: HDO (0 → 1995 cm-1)
- Kyuberis: H_2O (0.3 → 12796 cm-1), HDO (0. → 19935 cm-1)
- Regalia: H_2O (6452 → 9392 cm-1)/HDO (6451 → 9073 cm-1)

Evaluation of:

- ❑ HDO update
- ❑ H_2O update
- ❑ Impact of SDV

Validation of GEISA-2019 HDO

GEISA 2019 Update

- **Birk**: H_2O (1850 ➔ 4439 cm-1), HDO (**2478 ➔ 4439 cm-1**) Speed Dependent (SD) line profile
- **Coudert**: HDO (**0 ➔ 1995 cm-1**)
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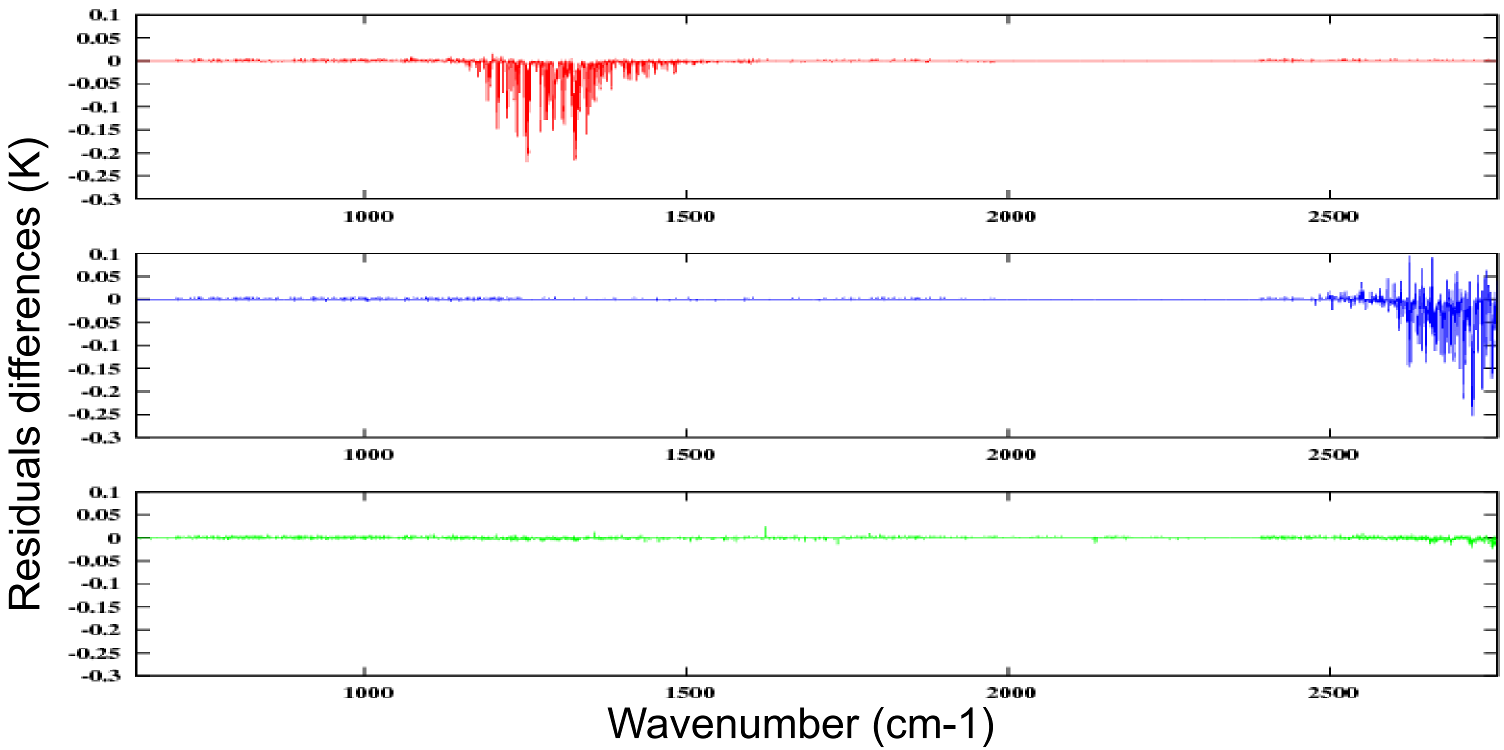
Evaluation of:

❑ **HDO update**



Validation of GEISA-2019 HDO

GEISA 2019 Update

- **Birk**: H_2O (1850 → 4439 cm-1), HDO (**2478 → 4439 cm-1**) Speed Dependent (SD) line profile
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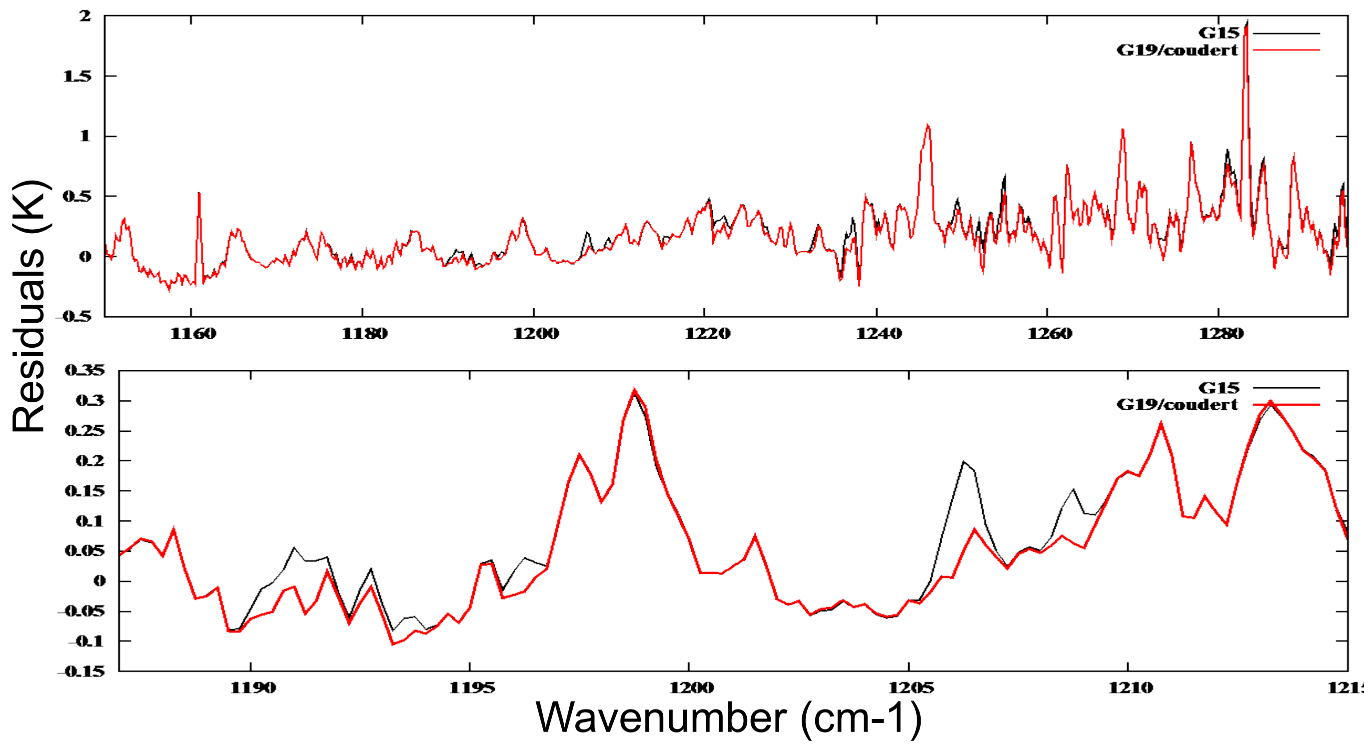
- Regalia: H_2O (6452 → 9392 cm-1)/HDO (6451 → 9073 cm-1)

Evaluation of:

- ❑ **HDO update**

Lower residuals with Coudert line list

→ Keep in GEISA-2019



Conclusion and *perspectives*

Since GEISA-2015, use of the SPARTE chain to evaluate the quality of Radiative Transfer modeling but also of spectroscopic parameters

- Cover the spectral ranges 645-2760; 4000-14000 cm-1
- Main molecules evaluate (H_2O, CO_2, O_3, N_2O, CO, CH_4 and O_2)
- Helpful for spectroscopic laboratories to prepare a better line list and for us in the finalization of the spectroscopic database
- Voigt profile

➔ Helpful in the preparation of GEISA-2019 planned for December 2019

- O_3
- CO_2 (Perevalov)
- HDO/H_2O (coudert, Birk)

- Evolution of SPARTE with over instruments (like ACE/FTS) to cover:
  - A better spectral range
  - More molecule

- Use other thermodynamical conditions than analyses and radiosoudings to reduce the collocation error:
  - O_3 radiosondes

- Evolution of GEISA and 4A/OP to non Voigt line profile parameters