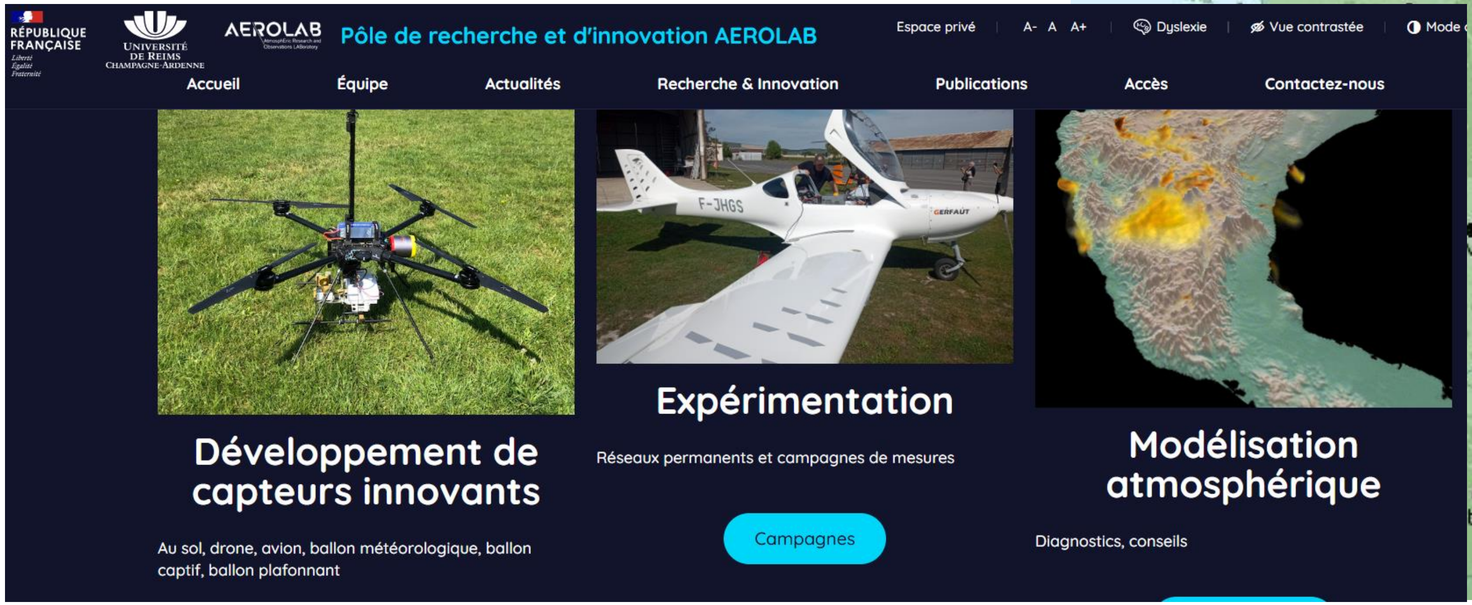
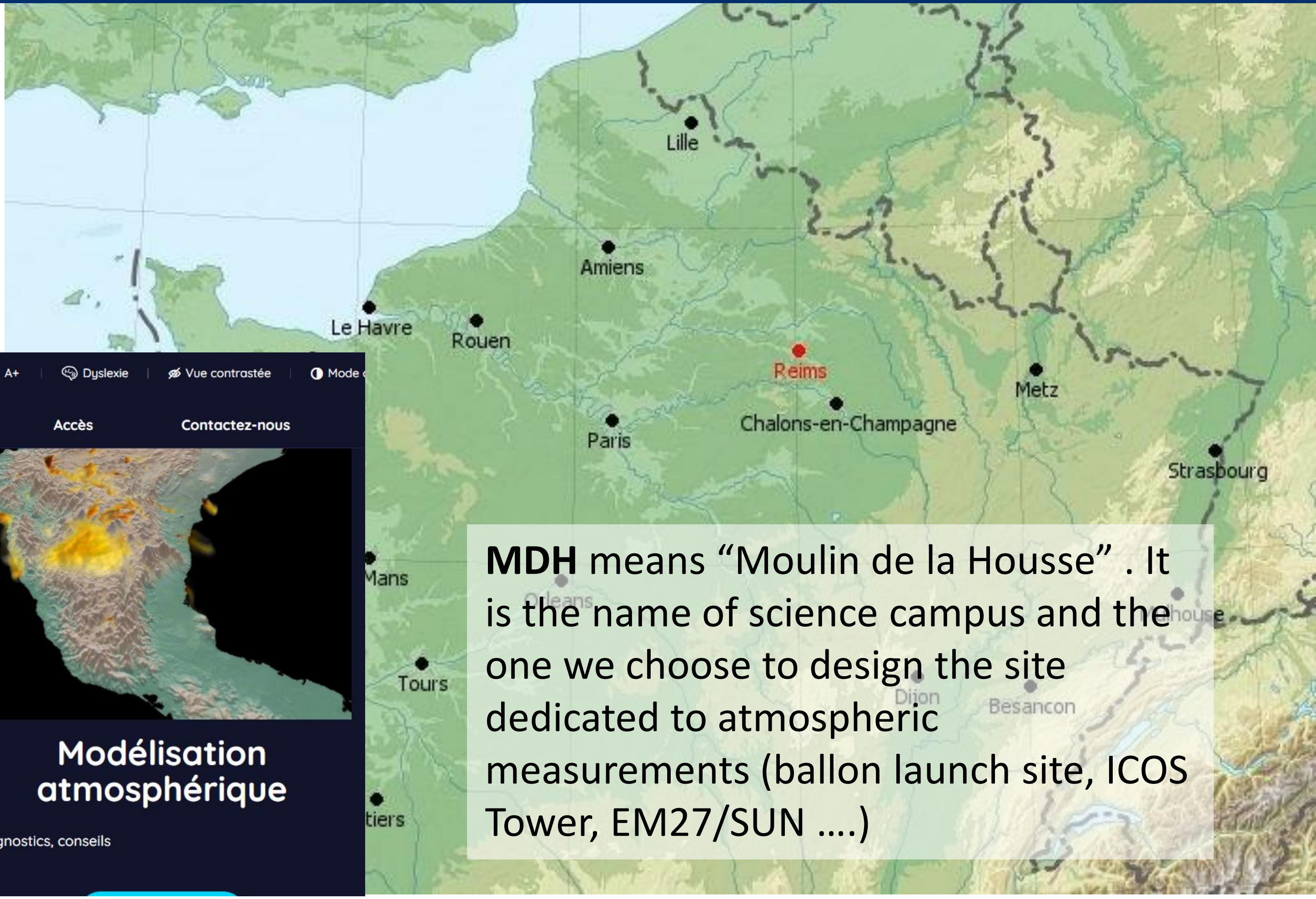
AEROLAB and « MDH » site @REIMS (France) 1/2

- AEROLAB = A research structure to provide expertise and solutions for monitoring and analyzing atmospheric emissions
- AEROLAB was born from the GSMA
- https://www.aerolab-innovation.com

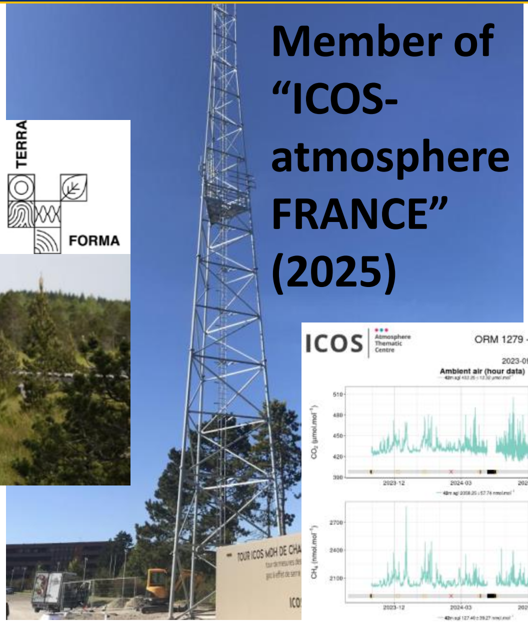




MDH means "Moulin de la Housse" . It is the name of science campus and the one we choose to design the site dedicated to atmospheric measurements (ballon launch site, ICOS Tower, EM27/SUN ….)

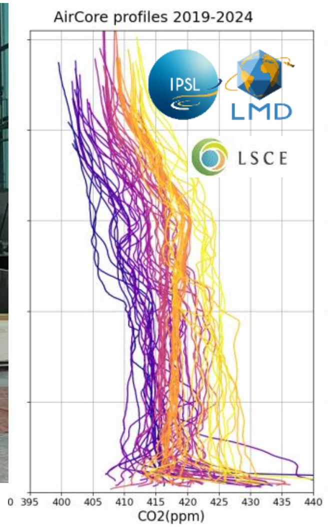
AEROLAB and « MDH » site @REIMS (France) 2/2

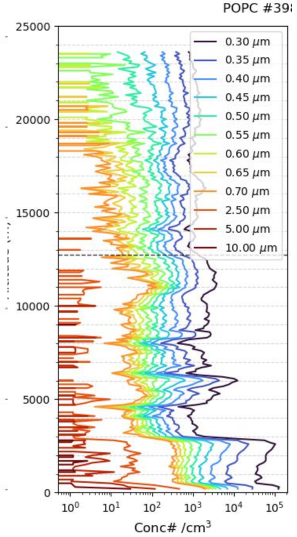
SURFACE



Member of "ICOS-atmosphere FRANCE" (2025)

ATMOSPHERIC





GHG (AirCore) + aerosol (POPC)

BALNEO Balloon Network

Nasa achievement award (2025)

https://science.larc.nasa.gov/balneo

Le Parisien

Des avions et des ballons au-dessus de Reims pour étudier la pollution atmosphérique

Depuis ce lundi 10 octobre, des avions et des ballons atmosphériques survolent la Cité des sacres. Pendant quinze jours ces manœuvres à basse ou haute altitude vont permettre de quantifier les émissions de gaz à effet de serre. Une cinquantaine de scientifiques du monde entier sont à Reims (Marne) pour cette campagne unique.

MAGIC

https://magic.aeris-data.fr/magic2022/#logbook

COLUMN

EM27/SUN begun in January 2020

Monitoring of greenhouse gases at the MDH location and assessment of the informative capabilities of the EM27/SUN with the ARAHMIS algorithm

Presented by : **EL HABCHI EL FENNIRI Hajar**

Context and Objectives of the Thesis

Scientific Context

- EM27/SUN spectrometers: key tools for calibration and validation of satellite GHG observations.Part of the European strategy for high-precision carbon monitoring (≈1 ppm, errors <0.5 ppm; Ciais et al., 2021).
- Thesis: use the ARAHMIS inversion model to analyze information content and identify sensitive spectral channels.

Objectives

- Investigate the information content of the EM27/SUN instrument.
- Propose potential improvements to PROFFAST or validate its current settings.
- Develop a unified inversion framework applicable to EM27/SUN data as well as satellite or other instruments (e.g., CHRIS).

[Ciais2015]: Ciais, P.; Crisp, D.; van der Gon, H.; Engelen, R.; Janssens-Maenhout, G.; Hiemann, M. & Rayner, P. Towards a European Operational Observing System to Monitor Fossil CO2 emissions– Final Report from the expert group European Commission Joint Research Centre, 2015

ARAHMIS Algorithm

Context:

- Developed at LOA (H. Herbin & F. Ducos)
- Reference code for space mission preparation:

IASI-NG, Biodiversity, FORUM, MicroCarb [1]

Collaboration:

- Access obtained during WS Magic 2023 (16/05/2023)
- Collaboration initiated with Prof. H. Herbin

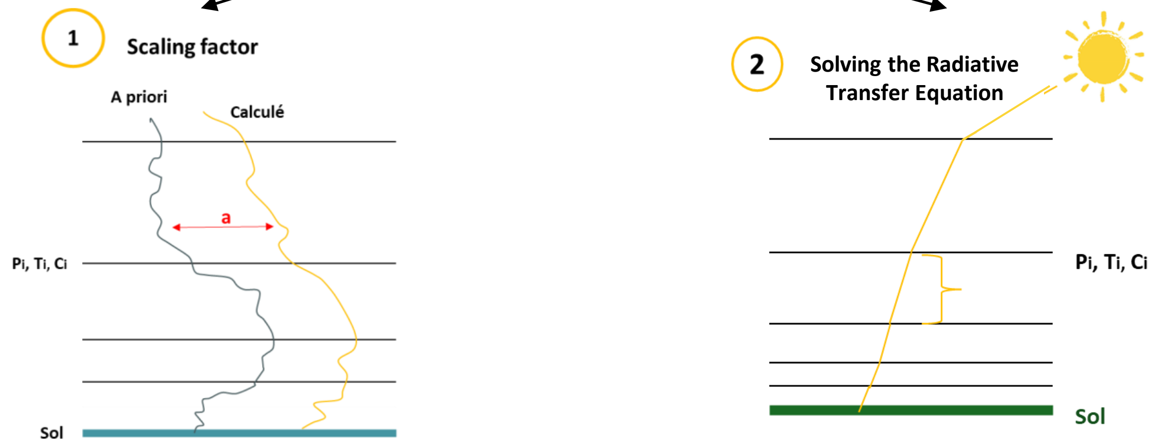
Operates in Two Steps :

ARAHMIS

Forward model

Retrieval

Inversion Method with ARAHMIS



Advantages	Drawbacks
SF & ETR	Requires Radiance Calibration
Inclusion of Aerosols	Time-consuming
Sandbox Mode – Adaptable to Observation Needs	! Spectrum Calibrated in Radiance !

[1]: Alalam, P., Ducos, F., & Herbin, H. (2024). Le rôle des indices de réfraction dans la mesure des poussières minérales avec des sondeurs satellites infrarouges à haute résolution spectrale : application au désert de Gobi. Chimie atmosphérique et physique , 24 (21), 12277-12294.

Steps to Achieve ARAHMIS

Radiance Calibration

Information Content Study

Channel Selection

Radiance Calibration

Radiance Calibration

Why calibrate?

- The EM27/SUN records FTIR spectra of direct solar radiation.
- High radiometric accuracy is required to retrieve reliable atmospheric column amounts (CO_2, CH_4, etc.).
- Calibration errors directly affect the quality of trace gas retrievals.

Current status (Transfer Function step):

- For now, the Transfer Function (TF) is performed using OPUS.

Method used:

- Method is based on the calculation of two parameters (Revercomb et al., 1988, adapted):

m (slope of the instrument response) & **b** (offset of the instrument response)

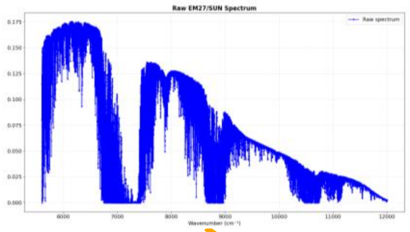
$$m = \frac{S_c - S_h}{B_\vartheta(T_c) - B_\vartheta(T_h)} \qquad b = \frac{S_c \,.\, B_\vartheta(T_h) - S_h \,.\, B_\vartheta(T_c)}{B_\vartheta(T_h) - B_\vartheta(T_c)}$$

S_c spectrum at **1523 K**, recorded using the LOA blackbody
S_h **EM27/SUN solar spectrum (maximum)**, recorded under optimal conditions (clean mirror, clear sky, solar noon).
$B_\vartheta(T_c)$ blackbody radiance at **1523 K**, calculated using Planck's law
$B_\vartheta(T_h)$ blackbody radiance at **6011 K**, from LATMOS (recent solar reference spectrum).

Calibrated solar spectrum:

$$L = \frac{S - b}{m}$$

Raw spectrum



m & b

Radiance spectrum

Input ARAHMIS

Blackbody Spectrum Recording – EM27/SUN

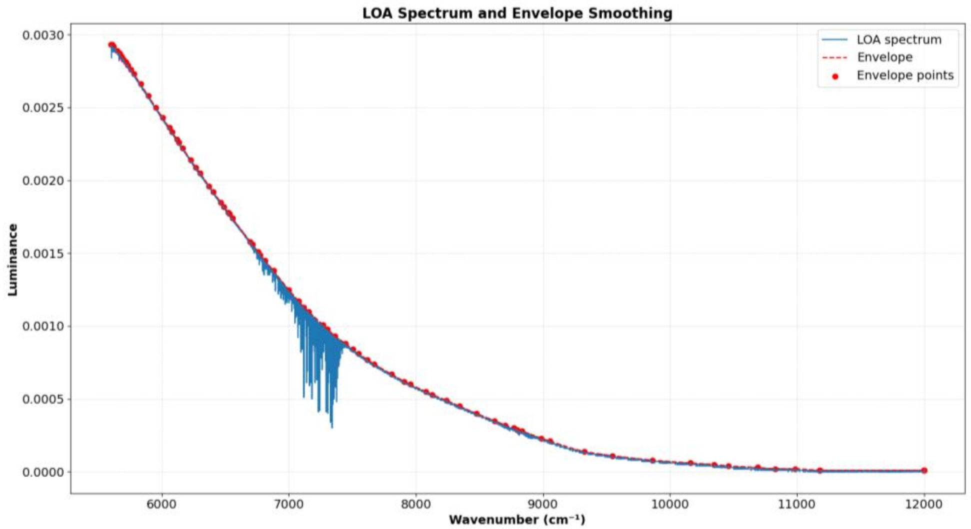
- Cold blackbody spectrum (1523 K) recorded at LOA with the EM27/SUN → used as reference (radiometrically calibrated)

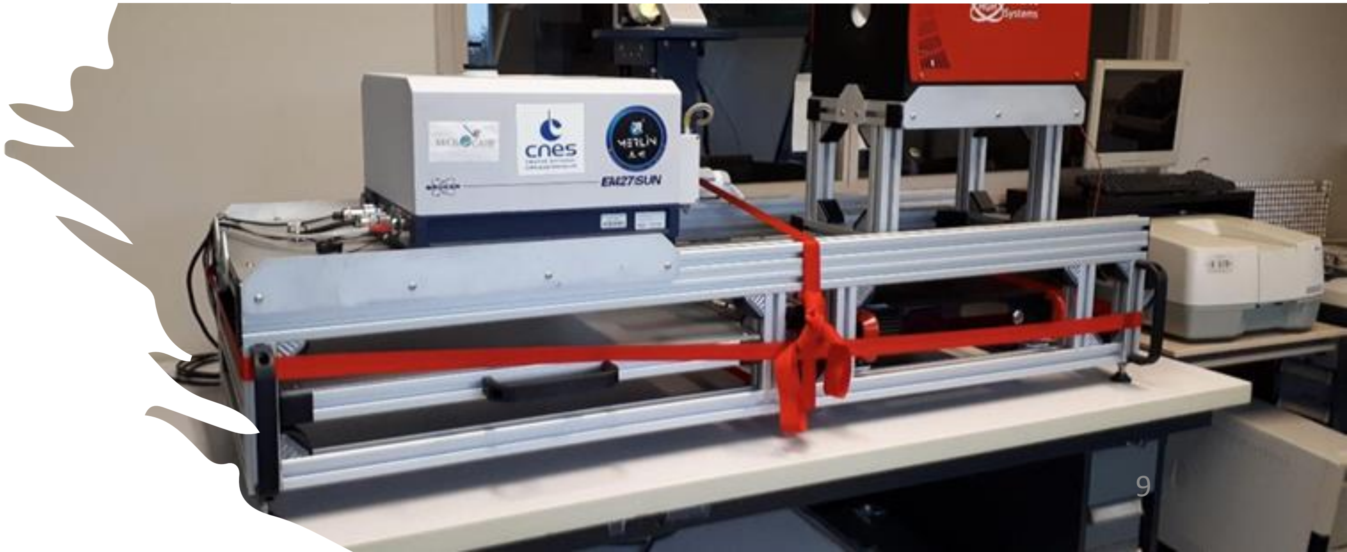
Processing of the 1523 K spectrum:

- Applied smoothing using an upper-envelope modeling approach.

Method:

- Manually selected control points.
- PCHIP interpolation (Piecewise Cubic Hermite Interpolating Polynomial) ➡ Code Python
- Advantages: Avoids oscillations & Preserves monotonicity of the data.





Solar Spectrum Correction and Smoothing

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Reference spectrum:

- The new solar spectrum from LATMOS (doi: 10.21413/SOLAR-V-DATABASE-SSI.L3.V1_SOLSPEC-LATMOS), measured by the SOLAR/SOLSPEC instrument on the ISS.

Attenuation at ground level:

- The solar spectrum is attenuated by: Rayleigh scattering (ROD) & Aerosols (AOD) (Casinière et al., 2005)

$$\boldsymbol{AOD = \cos(SZA)\ln\left(\frac{K_d I_{0\lambda}}{I_\lambda}\right) - ROD - k_0\Omega}$$

Assumptions:

- Seasonal Sun–Earth variation negligible $\rightarrow K_d = 1$
- NIR: ozone absorption negligible $\rightarrow k_0\Omega \approx 0$

Corrected spectrum:

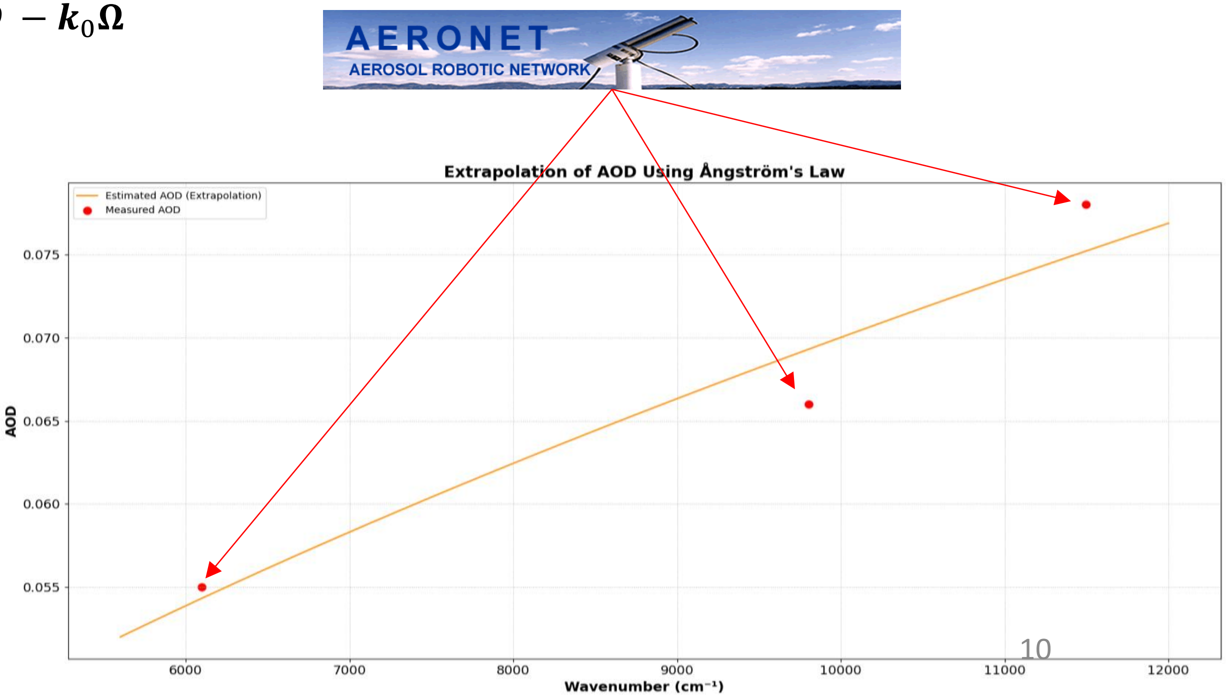
$$\boldsymbol{I_\lambda = I_{0\lambda}.\,e^{\left(-\frac{(AOD+ROD)}{\cos(SZA)}\right)}}$$

Rayleigh optical depth (ROD):

$$\mathbf{ROD = 0.008569(\lambda)^{-4}\,(1+0.0113(\lambda)^{-2}+0.00013(\lambda)^{-4})}$$

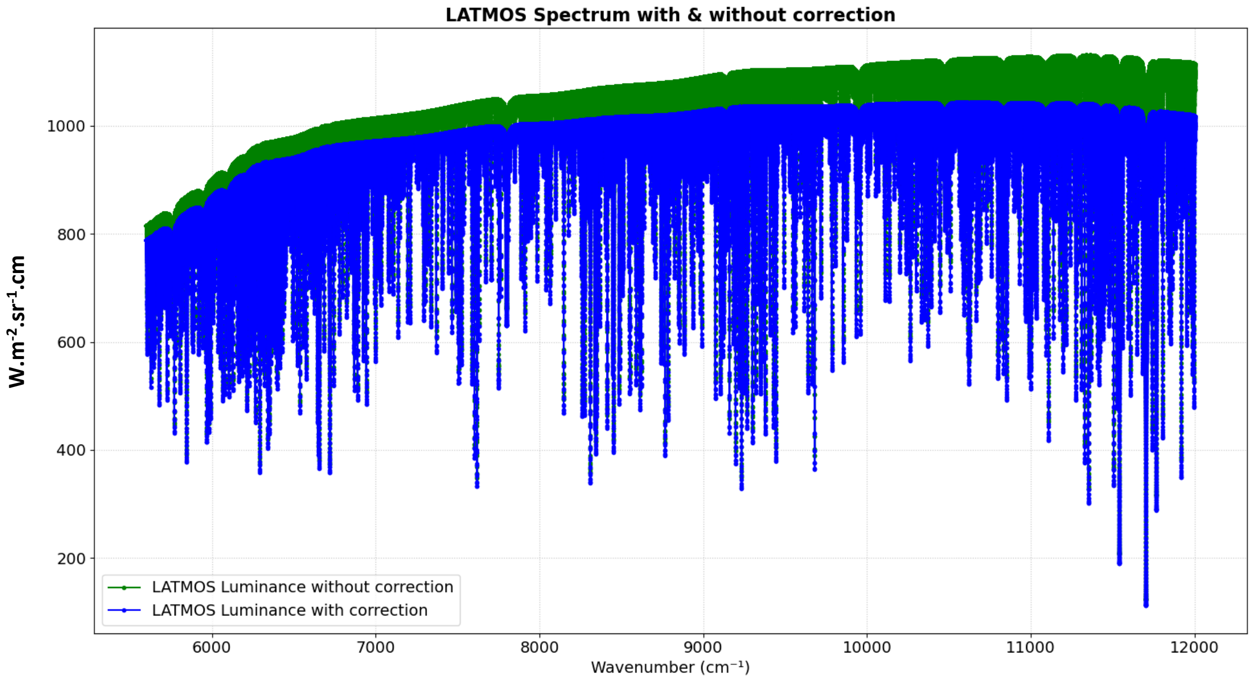
Aerosol Optical Depth (AERONET data: the three red points):

- Extrapolated using Ångström's law :

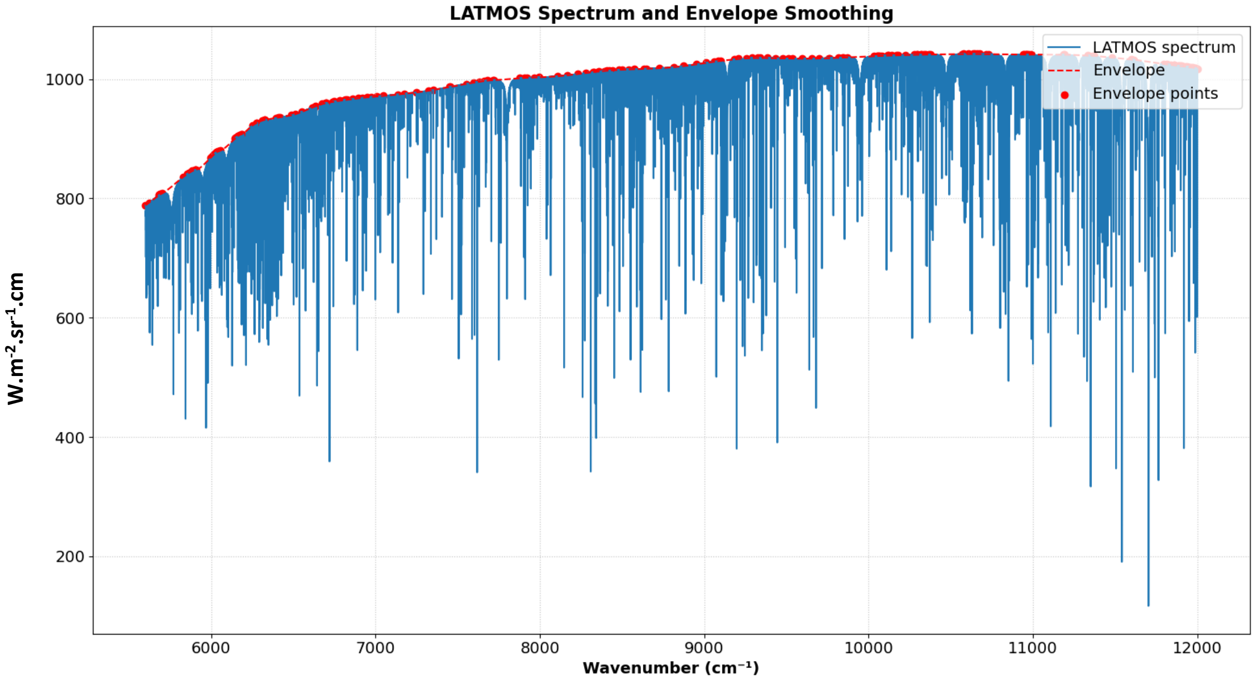


Solar Spectrum Correction and Smoothing

Comparison between solar spectrum before and after correction



Corrected spectrum with smoothing (PCHIP interpolation), same method as before



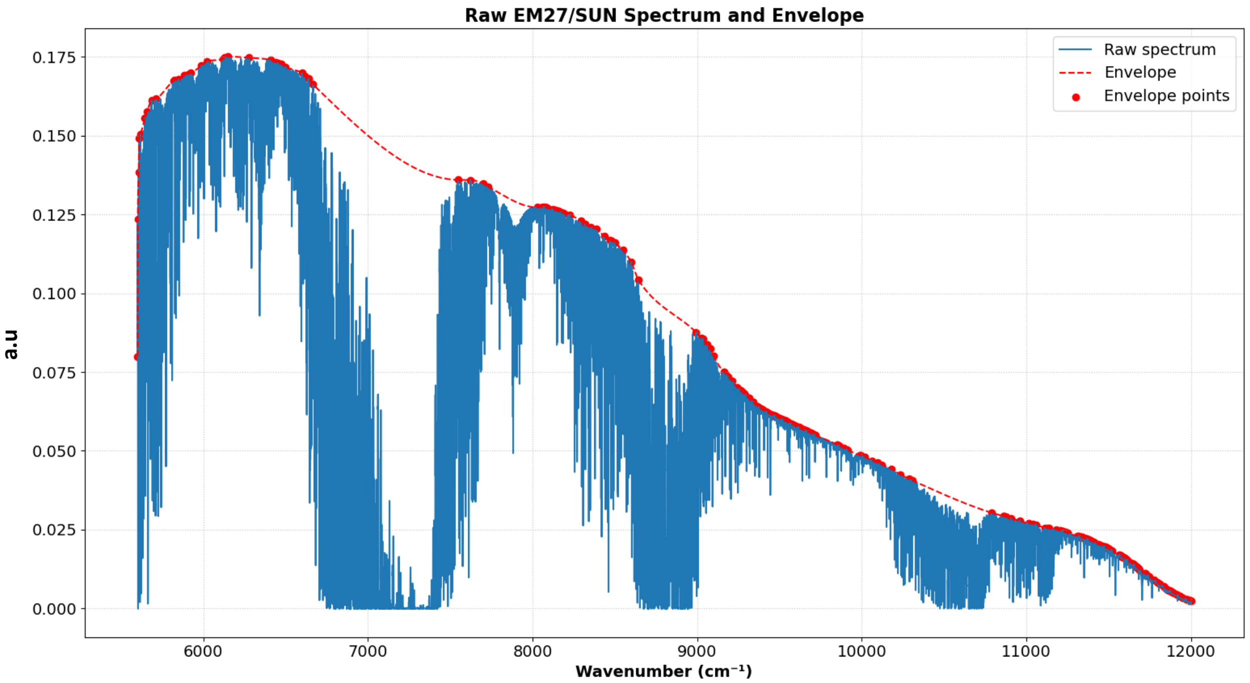
Selection of the EM27/SUN Spectrum

Acquisition conditions:

- Sunny day – June 13, 2023
- Selected spectrum: maximum recorded during the day

Processing applied:

- Spectre brut de l'EM27/SUN (Blue curve).
- Smoothing using PCHIP (red curve).



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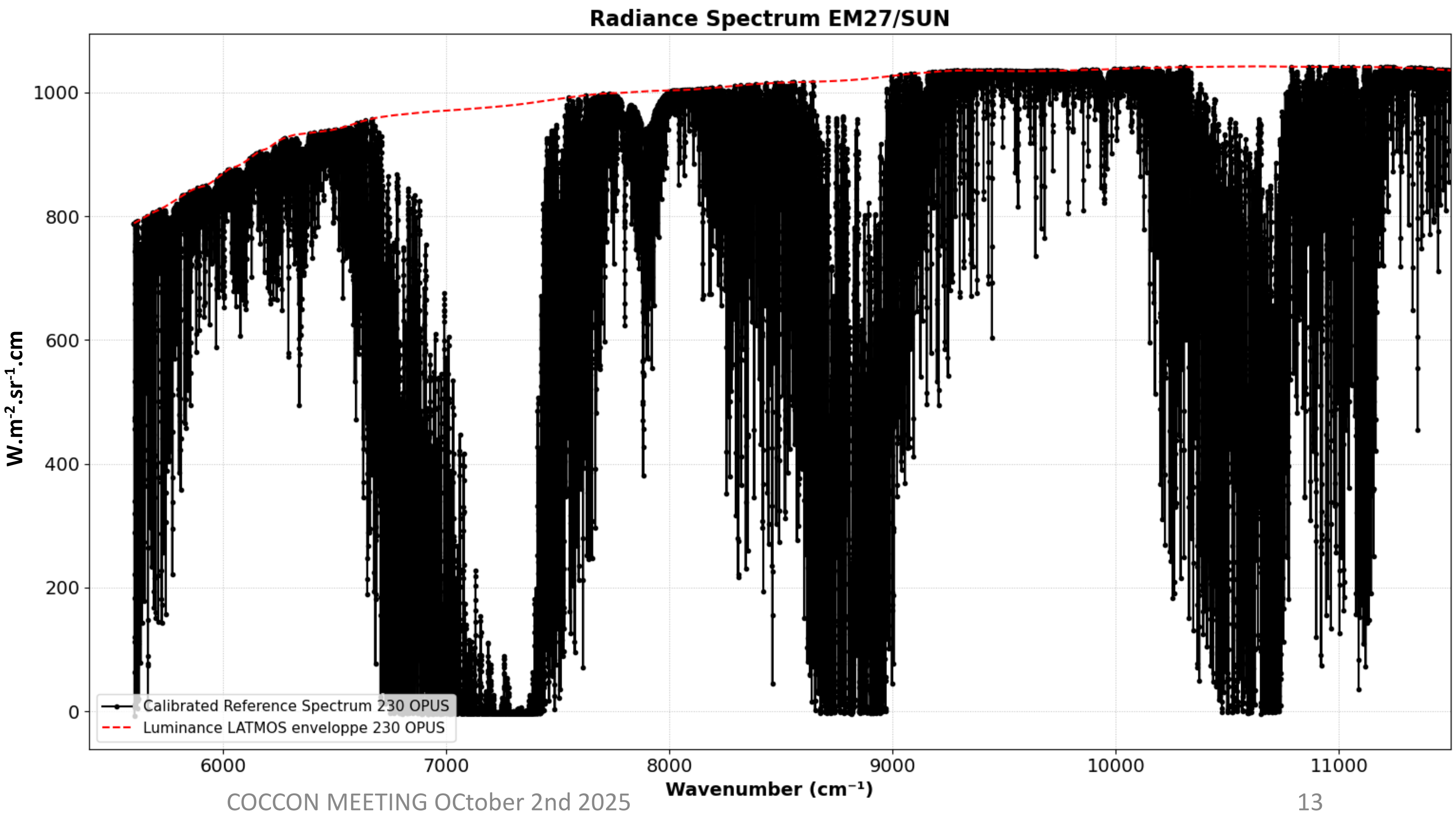
Calibrated Solar Spectrum – EM27/SUN

Final spectrum obtained after:

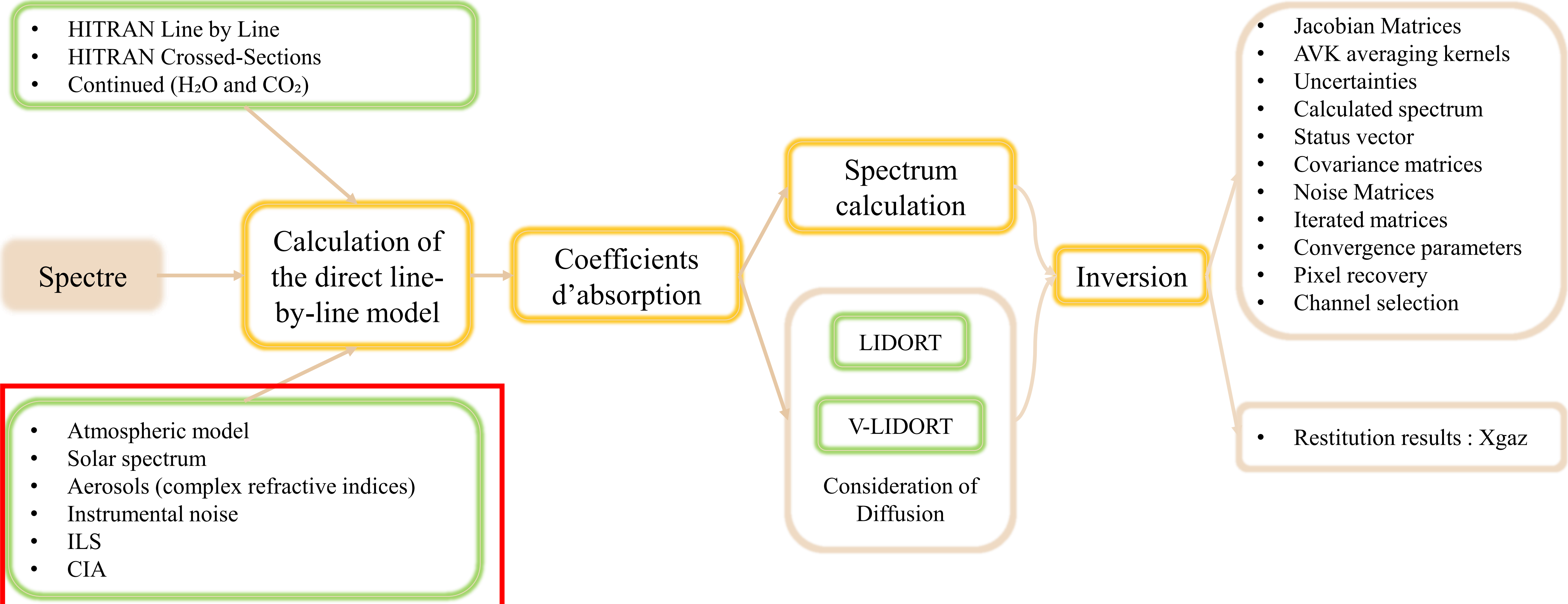
- Radiometric calibration (two-point method).
- Correction for Rayleigh scattering (ROD) and aerosols (AOD).
- Smoothing with PCHIP interpolation.

Spectrum is now ready to be used for ARAHMIS



Input Data for ARAHMIS

Input Data for ARAHMIS



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Adaptation of the GGG2020 Atmospheric Profile to ARAHMIS Requirements with In Situ Correction

Same a priori profile as PROFFAST

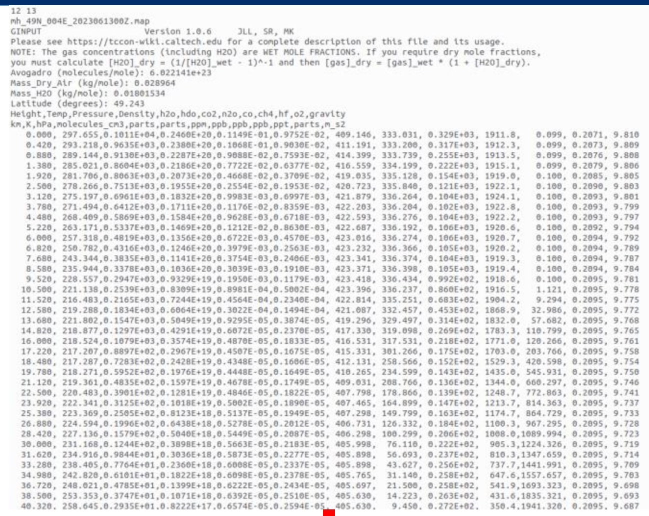
Ensures consistency in future comparisons (ARAHMIS vs PROFFAST)

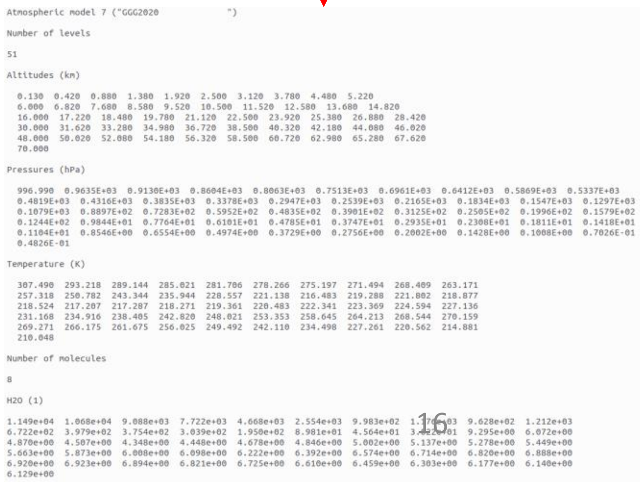
Development of a Restructuring Code

Converts GGG2020 profile (default format → ATM format)

Lowest layer

T & P replaced with in situ measurements (at spectrum time)





Noise Handling in ARAHMIS

Two options:

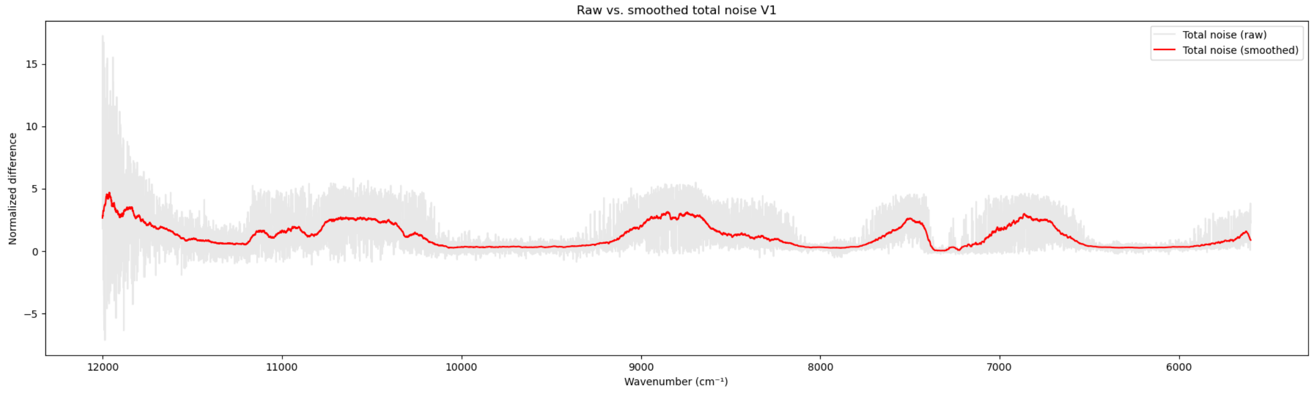
- Provide a single SNR value (fixed across the spectrum)
- Provide a noise profile file (wavenumber-dependent)

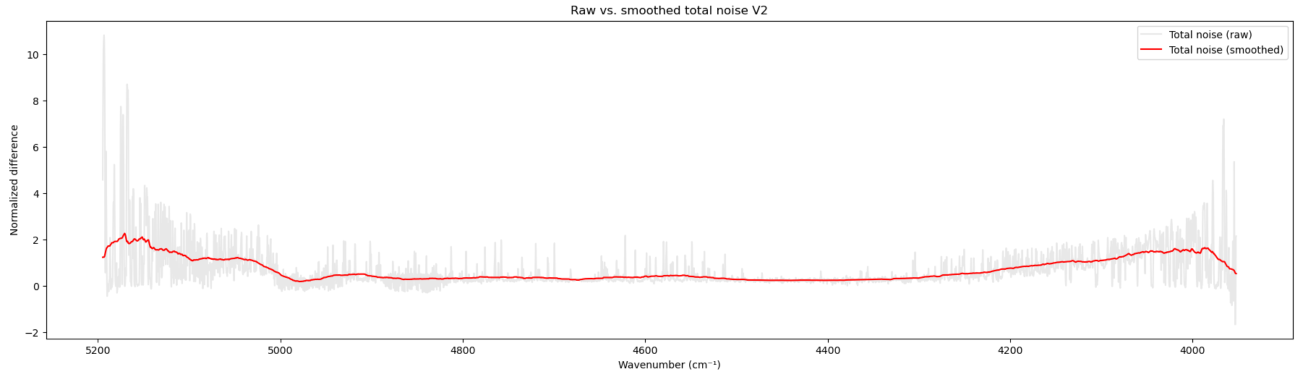
In this study:

Noise calculated for our instrument as:

$$Noise = \frac{std(S_1 - S_2)}{\sqrt{2}}$$

- Used directly as noise profile input in ARAHMIS





Instrument Line Shape (ILS) in ARAHMIS

ARAHMIS capabilities:

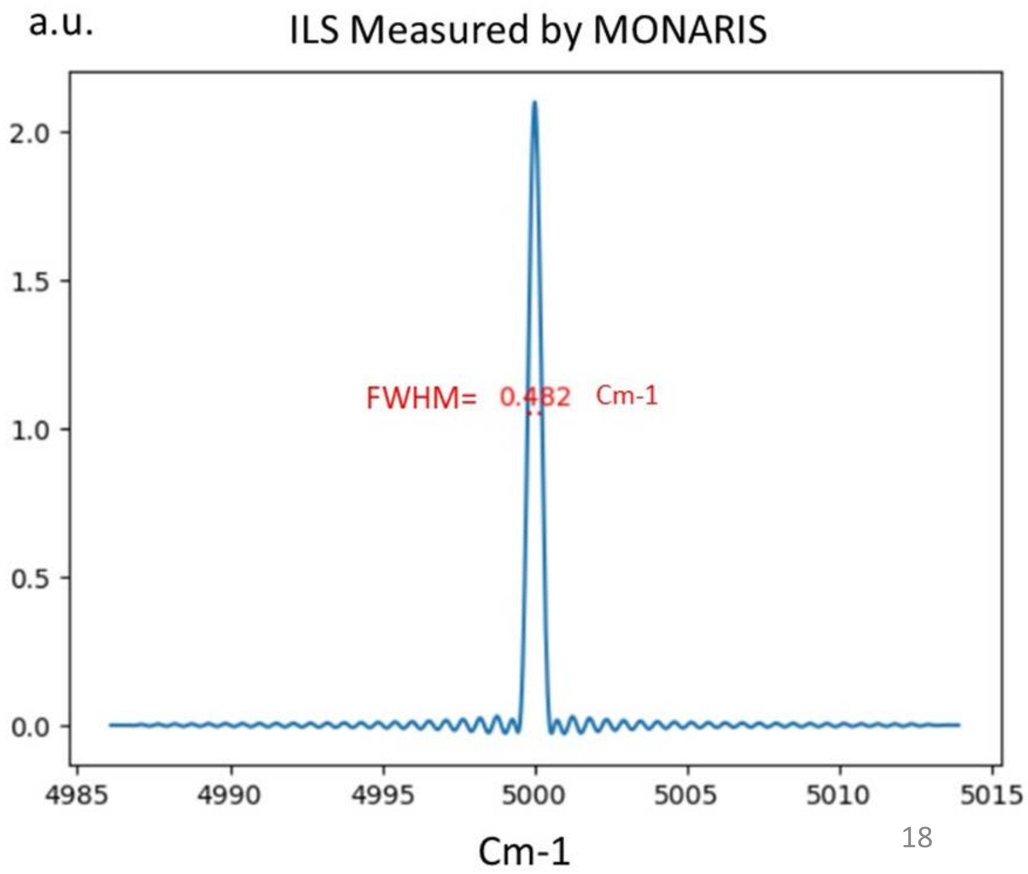
- Simulation of different apodization functions (sinc, gaussian, triangle, Lorentz, Norton-Beer weak, Norton-Beer medium, Norton-Beer strong Or direct ils file)

In this study:

- Measured **instrument ILS file** employed
- Extracted with **LINEFIT (v14.8)**
- Methodology: **Frey et al. (2015)**
- Modulation & phase parameters: **Alberti et al. (2022)**
- File provided by the **MONARIS team**

Application:

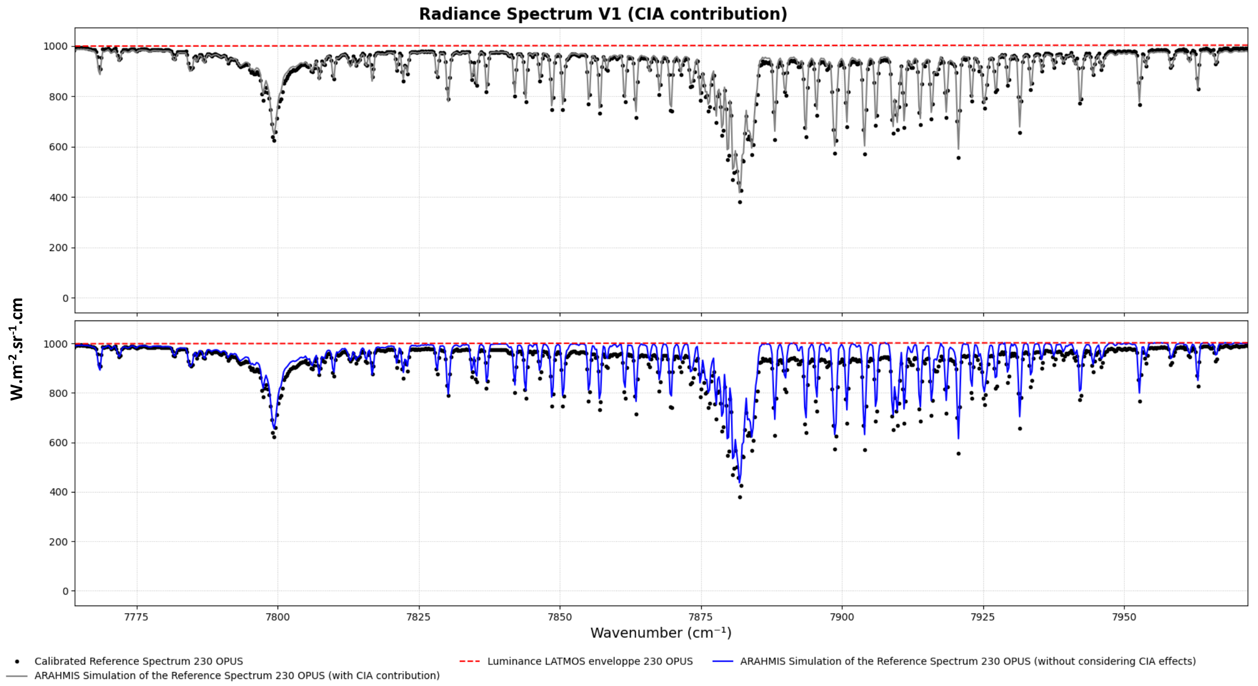
- Measured ILS used as **convolution kernel** in ARAHMIS
- Ensures accurate reproduction of observed spectra



Collision-Induced Absorption (CIA)

Definition / Importance

- Absorption due to transient dipoles created during molecular collisions.
- Crucial for an accurate simulation of measured spectra, especially in spectral regions affected by molecular interactions.
- Implemented in ARAHMIS according to the observation path used by EM27/SUN.



CIA Pairs Used

- Detector 1 (O_2): O_2–O_2, O_2–air
- Detector 2 (N_2): N_2–N_2, N_2–air

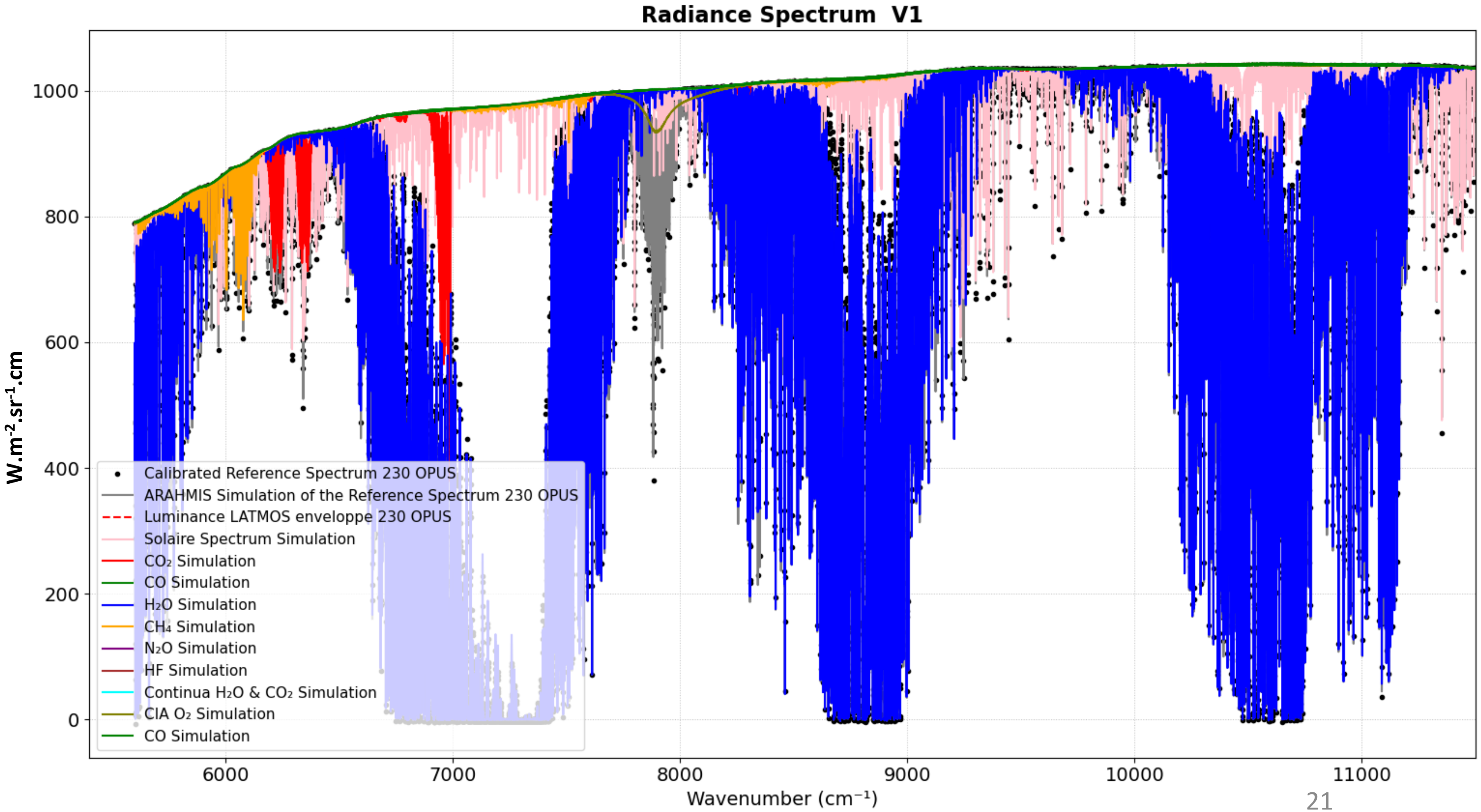
ARAHMIS Simulation

Comparison: Calibrated Spectrum vs ARAHMIS Simulation - Detector 1 (EM27/SUN)

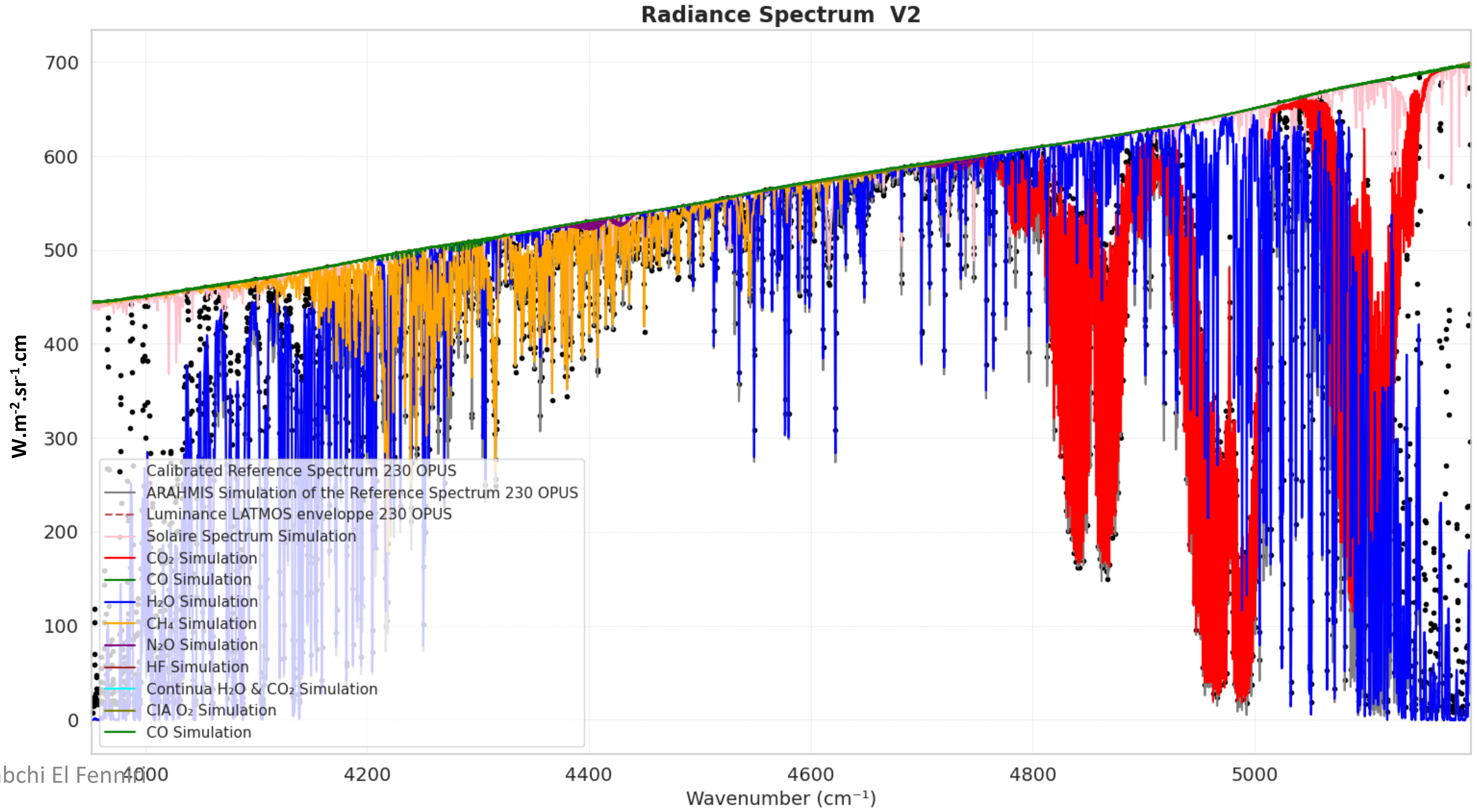
- Calibrated EM27/SUN spectrum
- ARAHMIS simulated spectrum (total)

Individual contributions:

- Molecular absorption (CO_2, H_2O, CH_4, O_2, …)
- CIA (Collision Induced Absorption)
- H_2O and CO_2 continua
- Solar reference spectrum



Comparison: Calibrated Spectrum vs ARAHMIS Simulation – Detector 2 (EM27/SUN)



Information Content Analysis

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Information Content Analysis – Rodgers (2000) Framework

General framework:

Rodgers' formalism (2000) quantifies the information content of measurements and the associated uncertainties.

The analysis is based on (for more details, see chapter 3 of [Rodgers(2000)] C D Rodgers. Inverse Methods for Atmospheric Sounding. WORLD SCIENTIFIC, 2000.):

- Averaging Kernel (AVK) matrices.
- Different error sources in the retrieval.

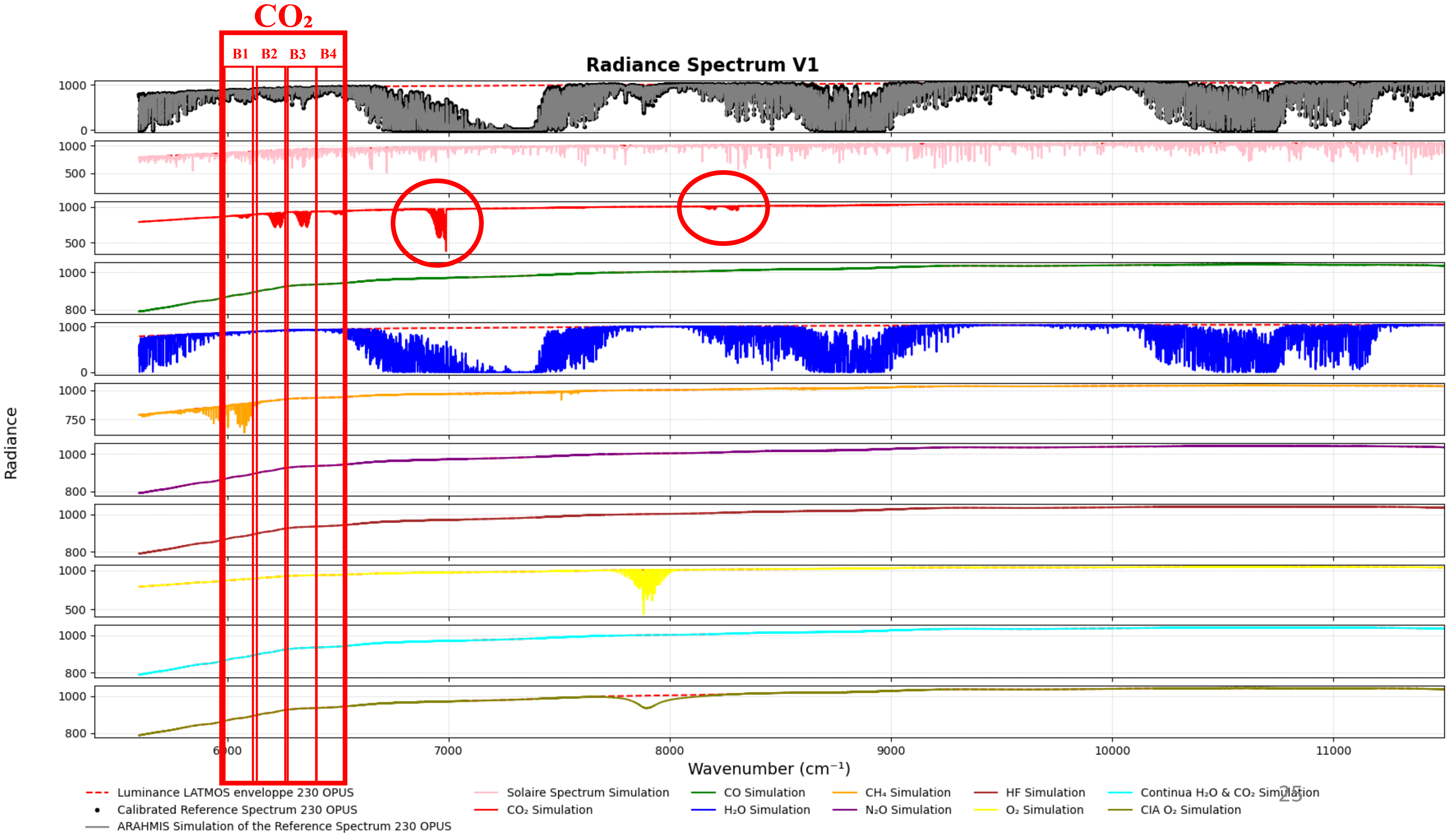
Error sources considered:

- **Smoothing error**: due to the influence of the a priori on the retrieved profile.
- **Model error**: approximations in the radiative transfer representation.
- **Measurement error**: instrumental uncertainties and measurement noise.
- **A priori error**: linked to the choice of the assumed initial profile.

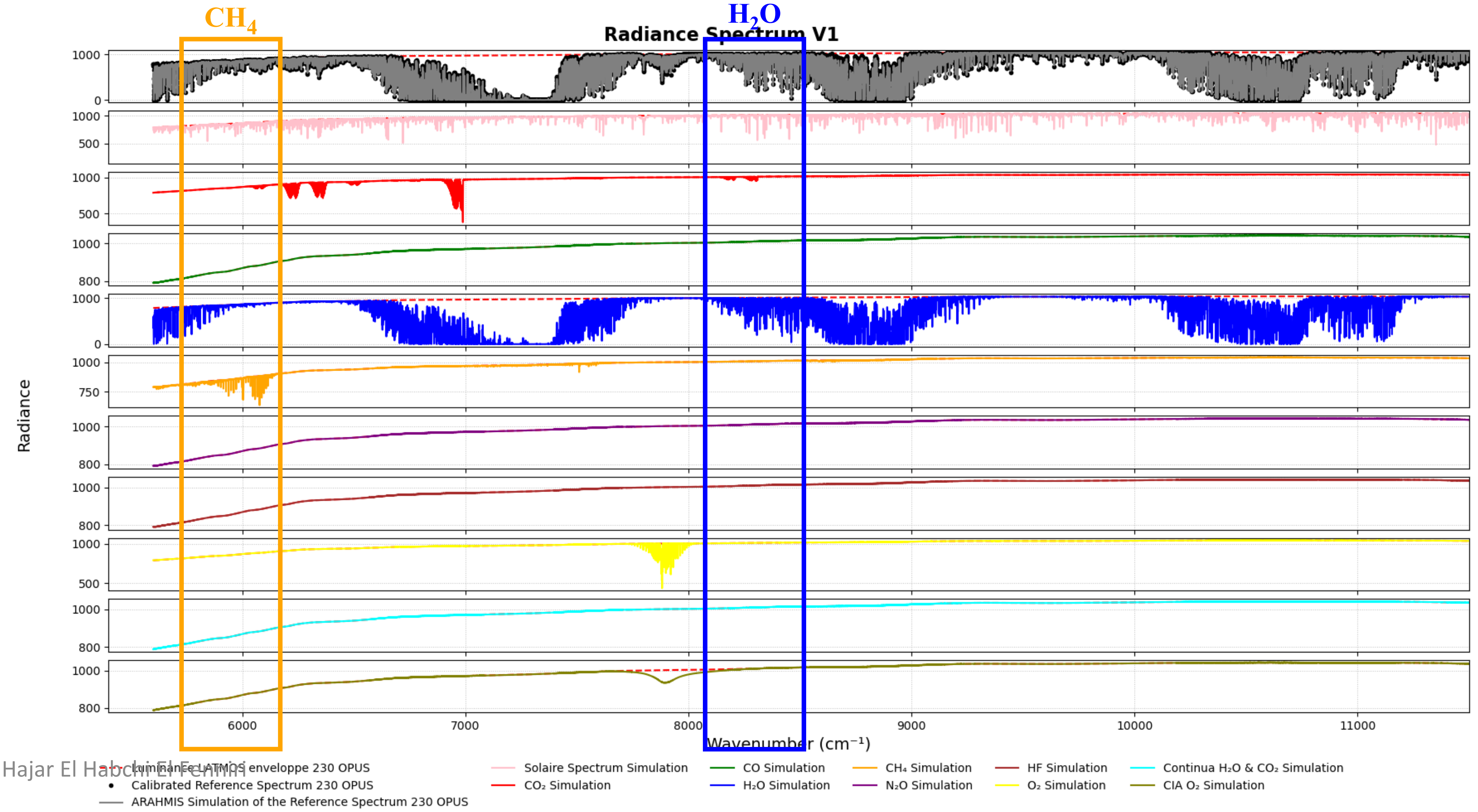
Identification of Absorption Features – ARAHMIS Simulation - Detector 1 (EM27/SUN)

Objective:

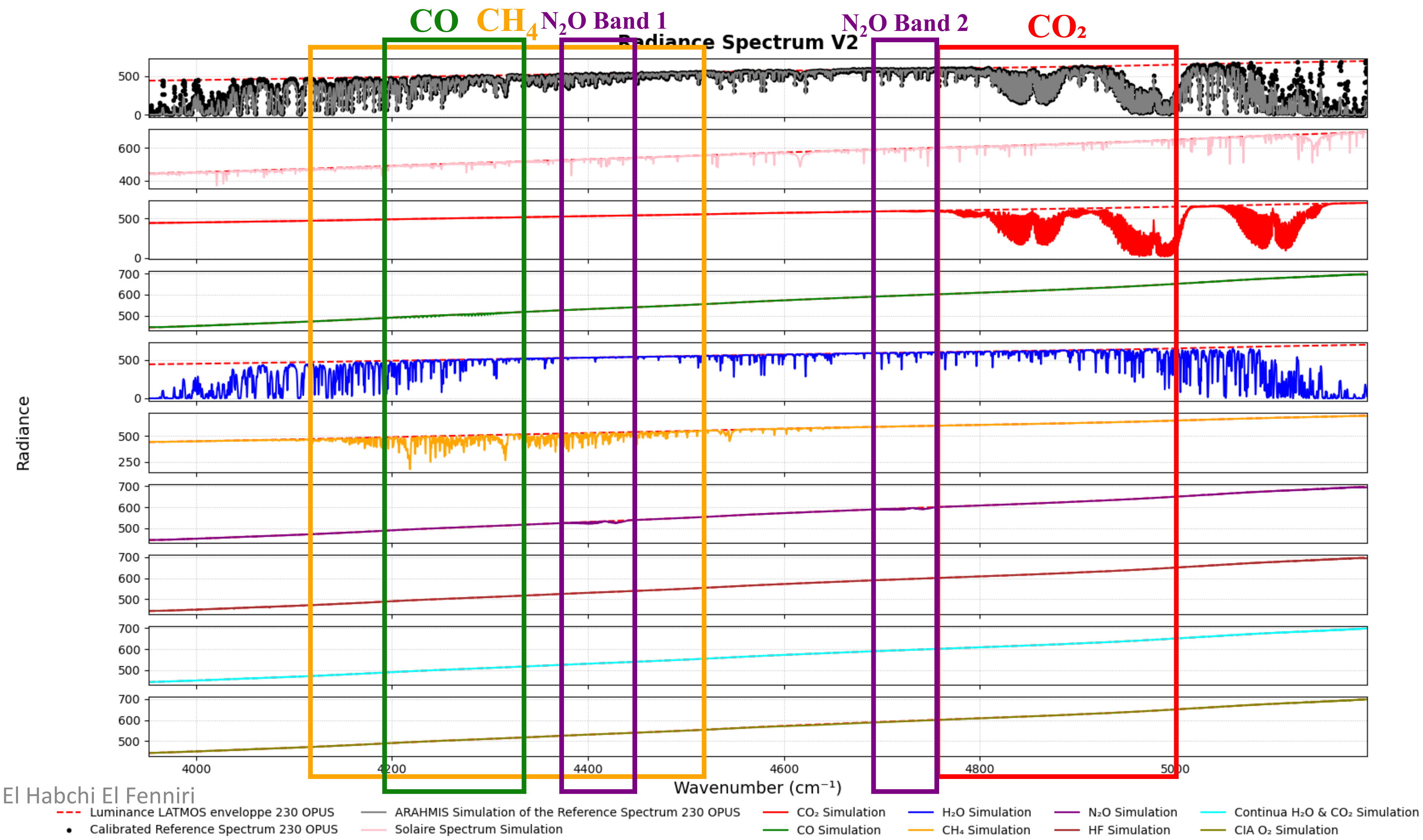
- Identify absorption bands of each molecule.
- Detect overlapping regions where several species absorb simultaneously.



Identification of Absorption Features – ARAHMIS Simulation - Detector 1 (EM27/SUN)



Identification of Absorption Features – ARAHMIS Simulation - Detector 2 (EM27/SUN)



Summary of Entries

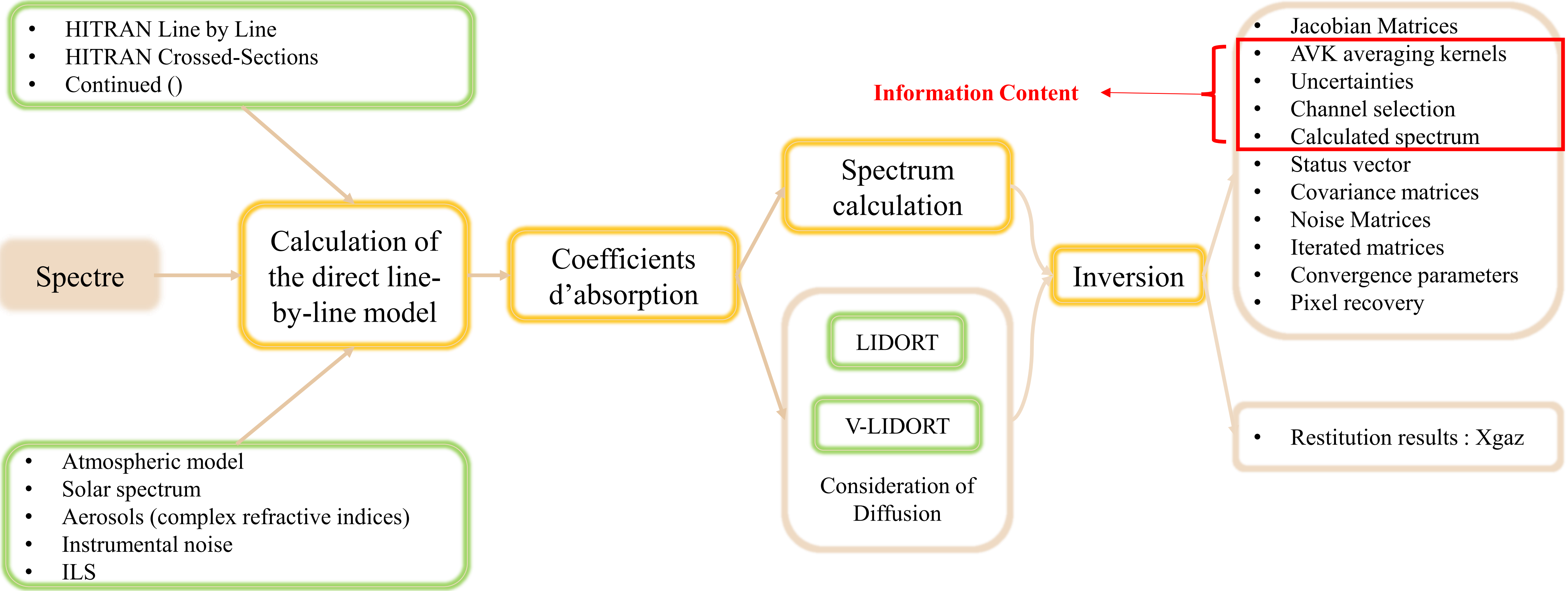
Detector 1 :

		A priori	CIA O_2–O_2, O_2–air	Noise	ILS	Solar Spectrum Correction	H_2O	CO_2	CH_4
CO_2	Band 1 : 6038.21709, 6107.88233	✓	✓	✓	✓	✓	✓	✓	✓
CO_2	Band 2 : 6166.21794, 6259.02458	✓	✓	✓	✓	✓	✓	✓	
CO_2	Band 3 : 6293.01351, 6379.79374	✓	✓	✓	✓	✓	✓	✓	
CO_2	Band 4 : 6463.92236, 6533.82866	✓	✓	✓	✓	✓	✓	✓	
CH_4	Band : 5741.2358, 6170.0748	✓	✓	✓	✓	✓	✓	✓	✓
H_2O	Band : 8318.12676, 8598.2340	✓	✓	✓	✓	✓	✓		

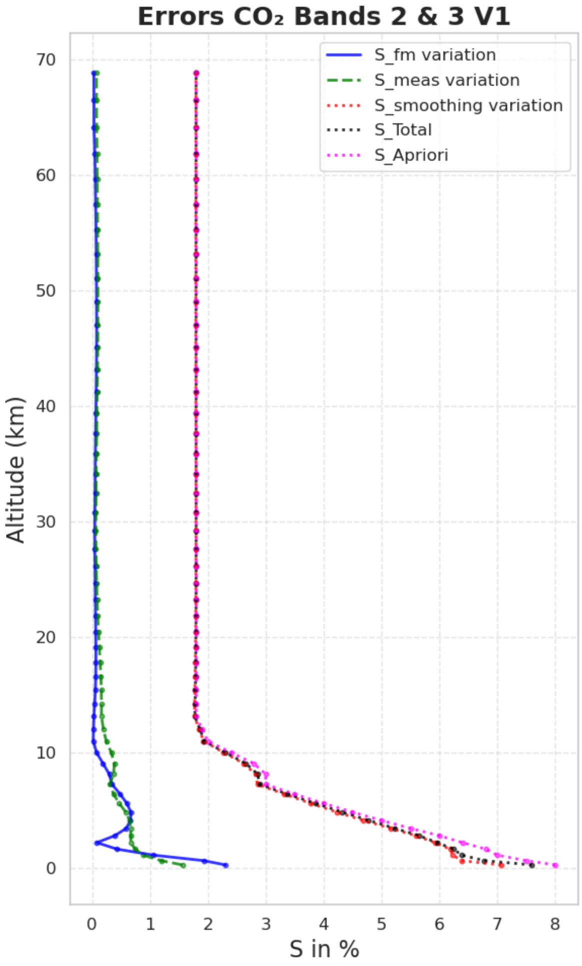
Detector 2 :

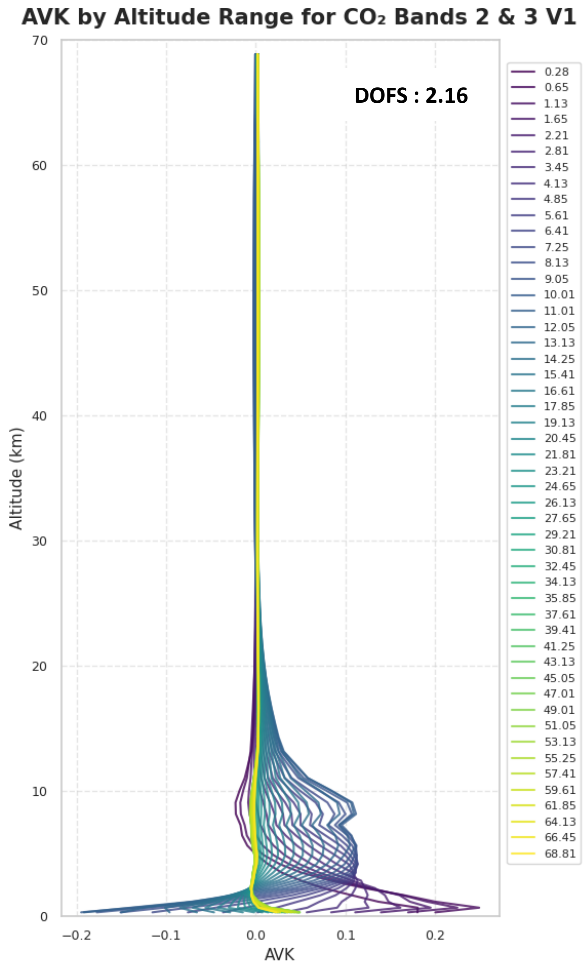
		A priori	CIA N_2–N_2, N_2–air	Noise	ILS	Solar Spectrum Correction	H_2O	CO_2	CH_4	CO	N_2O
CO_2	Band : 4722.0501, 5002.1574	✓	✓	✓	✓	✓	✓	✓			✓
CH_4	Band : 4179.1915, 4675.7673	✓	✓	✓	✓	✓	✓		✓	✓	✓
CO	Band : 4187.1464, 4326.9590	✓	✓	✓	✓	✓	✓		✓	✓	
N_2O	Band 1 : 4371.0723, 4442.9070	✓	✓	✓	✓	✓	✓		✓		✓
N_2O	Band 2: 4699.14982, 4756.7622	✓	✓	✓	✓	✓	✓	✓			✓

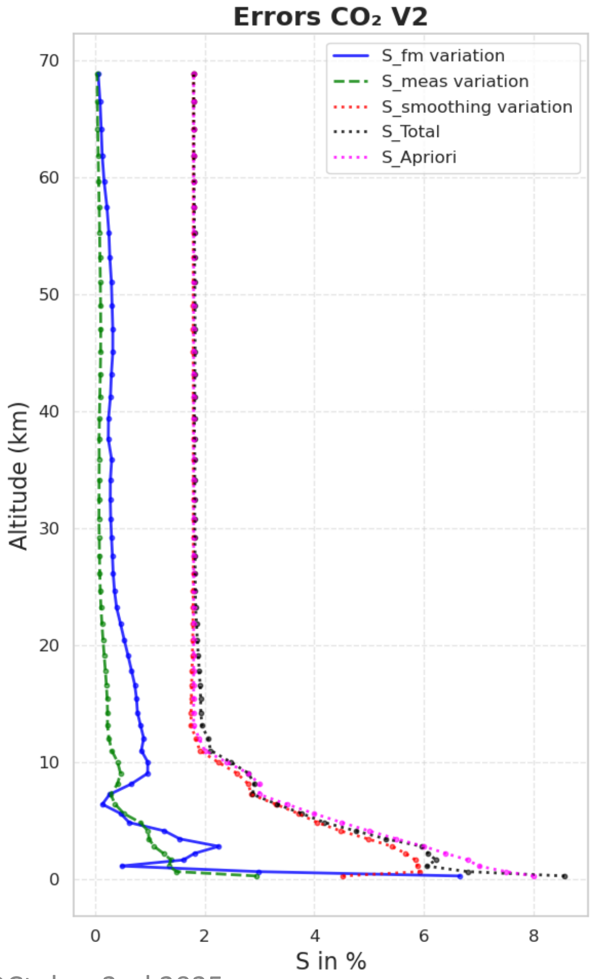
Output Data for ARAHMIS

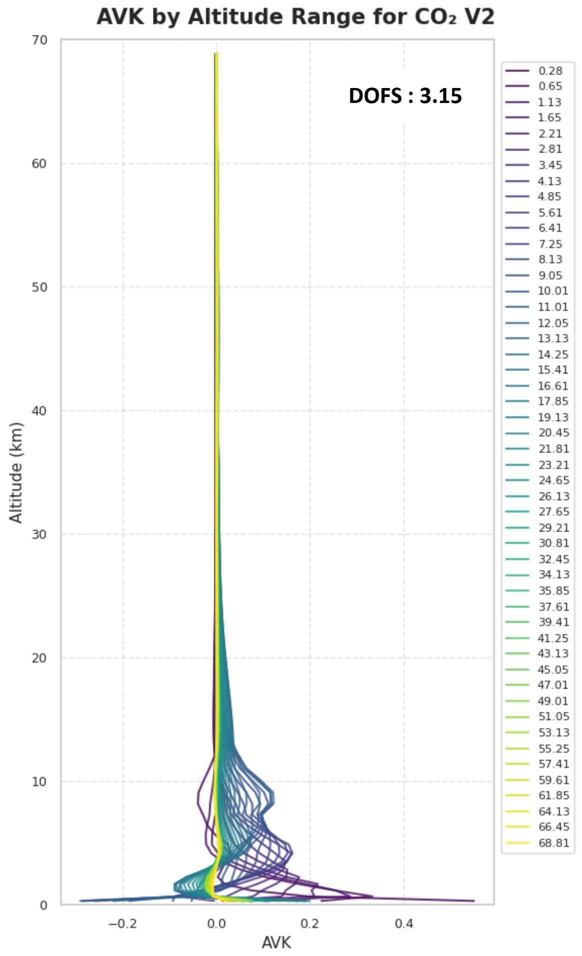


Example Plots of Errors and AVKs









Summary of DOFS and Errors

- Detector 1: the combination of bands 2 & 3 represents an optimal compromise:
  - Provides as much information as using all 4 bands (DOFS ≈ 2.16 vs 2.22).
  - AVKs and posterior errors are nearly identical → no significant loss of quality.
  - Reduces computation time and avoids spectral redundancy.
- Detector 2: more performant (DOFS = 3.15) → provides greater independent information.
- Sensitivity altitude: EM27/SUN is mainly sensitive to CO_2 in the lower troposphere, consistent with its use for total column monitoring.
- Dominant error: smoothing error → highlights the importance of a robust a priori.

	CO_2					
	Band	DOFS	Smoothing uncertainty		Total Error	
			S_smoot % max	Altitude	S_total % max	Altitude
Detector 1	Band 1 : 6038.21709, 6107.88233	1,01	7.750120	0.28	7.858250	0.28
Detector 1	Band 2 : 6166.21794, 6259.02458	1,93	7.18440	0.28	7.53491	0.28
Detector 1	Band 3 : 6293.01351, 6379.79374	1,90	7.20534	0.28	7.51155	0.28
Detector 1	Band 4 : 6463.92236, 6533.82866	0,98	7.756640	0.28	7.936460	0.28
Detector 1	Bands 1 et2	1,98	7.19798	0.28	7.61311	0.28
Detector 1	Bands 2 et 3	**2,16**	7.07130	0.28	7.59874	0.28
Detector 1	Bands 3 et 4	1,94	7.20179	0.28	7.55248	0.28
Detector 1	Bands 1 à 4	2,22	7.05730	0.28	7.72628	0.28
Detector 2	Band : 4722.0501, 5002.1574	**3,15**	5.93085	0.65	8.56782	0.28

Summary of DOFS and Errors

- Detector 2 is clearly more efficient for CH_4:
  - Higher DOFS (2.30 vs 1.82).
  - Sensitivity concentrated in the lower troposphere, more suitable for monitoring surface emissions.

CH_4						
	Band	DOFS	Smoothing uncertainty		Total uncertainty	
			S_smoot % max	Altitude	S_total % max	Altitude
Dedector 1	Band : 5741.2358, 6170.0748	1,82	5	51.05	5.030900	17.85
Detector 2	Band : 4179.1915, 4675.7673	**2,30**	5	53.13	5.039280	0.28

- High information content (DOFS = 2.5) with strong sensitivity in the lower troposphere.
- Stable errors (~5%) → EM27/SUN provides robust retrievals of water vapor.

- Very limited information (DOFS = 0.37).
- Absorption lines are too weak, as clearly confirmed in the simulations.
- Although CO retrievals are often mentioned in the literature, these results show that EM27/SUN provides poor sensitivity for CO.

- Provides non-negligible information (DOFS ~0.9), with sensitivity in both the lower and upper troposphere.
- N_2O retrievals from EM27/SUN have not been addressed in the literature

		Band	DOFS	Smoothing uncertainty		Total Error	
				S_smoot % max	Altitude	S_total % max	Altitude
Detector 1	H_2O	Band : 8318.12676, 8598.2340	**2,5**	5.000040	13.13	5.000470	7.25
Detector 2	CO	Band : 4187.1464, 4326.9590	**0,37**	5	35.85	5.37858	0.65
Detector 2	N_2O	Band 1 : 4371.0723, 4442.9070	**0,94**	5	35.85	5	34.13
Detector 2	N_2O	Band 2 : 4699.14982, 4756.7622	0,69	5	34.13	5.101910	2.21

Construction of the A Priori Covariance Matrix

Objective:

- Provide an a priori profile together with its variance and covariance matrix (including vertical correlations).
- In ARAHMIS, this matrix goes beyond variance: It introduces covariance, linking the levels and allowing the inversion to optimally weight information from both the a priori and the measurements.

Principle:

- Use AirCore profiles as the basis.
- AirCore data limited to 20–25 km altitude.
- Completed with CAMS outputs to extend up to 70 km (EM27/SUN grid).

Methodology:

- Constructed from 19 days of data around the reference date:
  - ✓ June 13, 2023 (day of the studied spectrum).
- Provides a realistic representation of atmospheric variability during the study period.

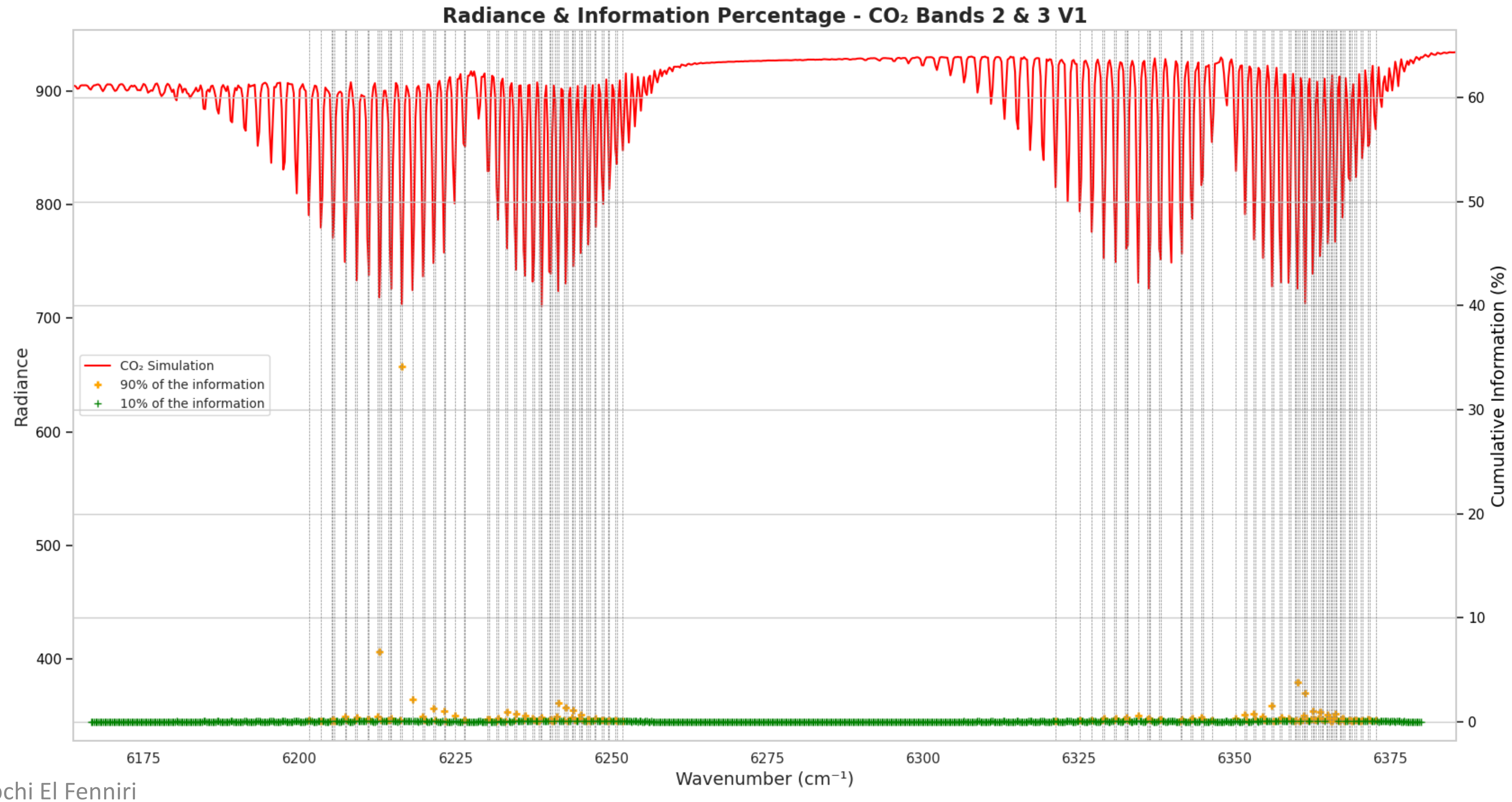
Summary of DOFS with and without the covariance matrix

- Covariance significantly reduces DOFS → much of the raw information is redundant.
- Detector 2 remains more efficient, especially for CH_4.
- Sensitivity shifts upward, reducing constraints near the surface.
- CH_4 retains more independent information than CO_2, even with covariance.

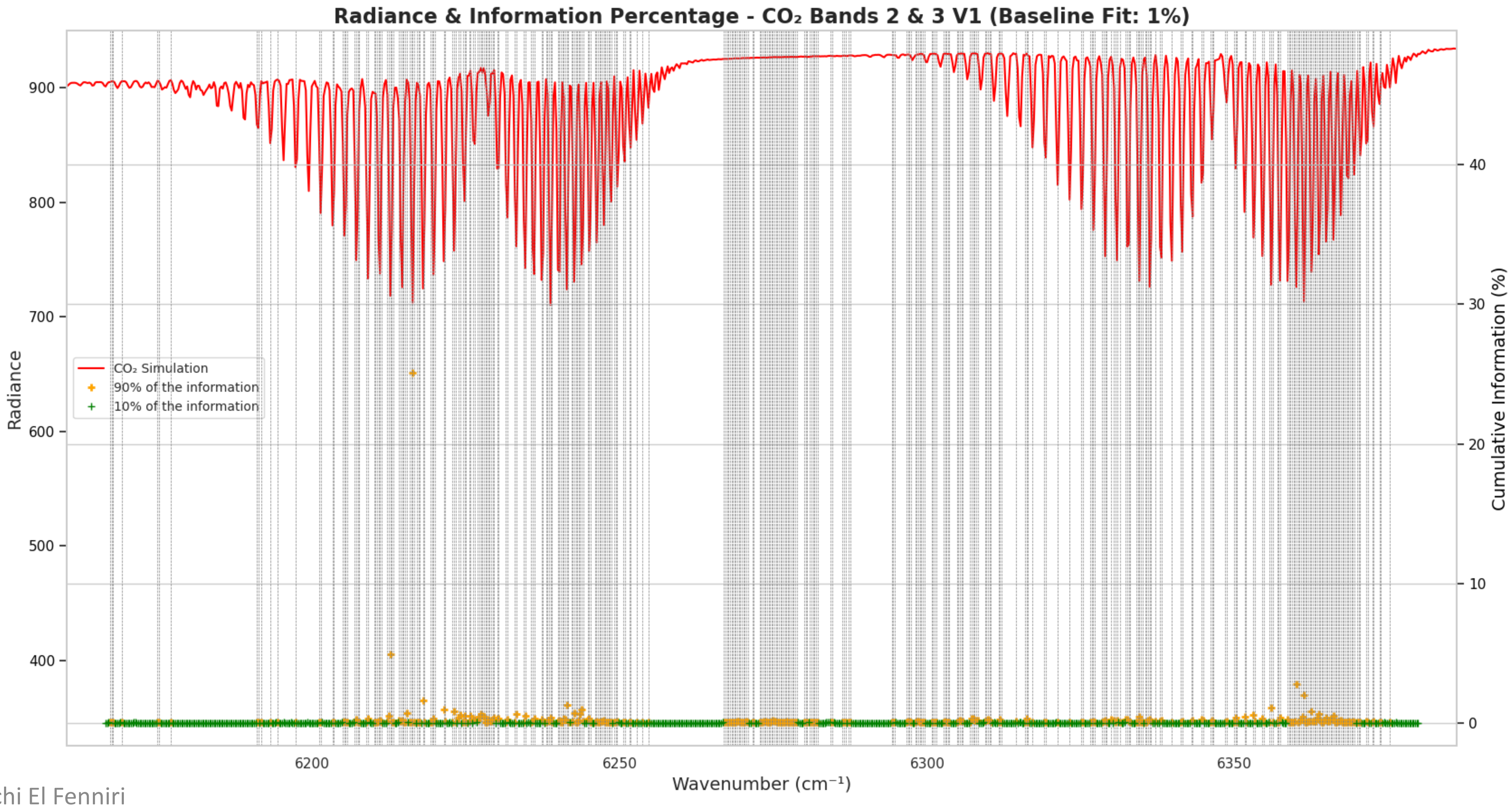
		Without covariance matrix			With covariance matrix		
	Fenêtre	DOFS	S_smoot % max	Altitude	DOFS with Covariance	S_smoot % max	Altitude
Detector 1	**CO2**						
	Fenêtre 1 : 6038.21709, 6107.88233	1,01	7.750120	0.28	0,440	3.26277	0.275
	Fenêtre 2 : 6166.21794, 6259.02458	1,93	7.18440	0.28	0,979	1.88078	13.13
	Fenêtre 3 : 6293.01351, 6379.79374	1,90	7.20534	0.28	0,980	1.88071	13.13
	Fenêtre 4 : 6463.92236, 6533.82866	0,98	7.756640	0.28	0,508	2.91026	0.275
	Fenêtre 2 et 3	2,16	7.07130	0.28	0,997	1.87477	13.13
	CH4						
	Fenêtre : 5741.2358300, 6170.07483765	1,82	5	51.05	1,099	0.06545	21.81
Detector 2	**CO2**						
	Fenêtre CO2	3,15	5.93085	0.65	1,047	1.82914	13.13
	CH4						
	Fenêtre CH4	2,30	5	53.13	1,424	0.060426	21.81

Channel Selection

Channels and corresponding percentages



Channels and corresponding percentages



Summary of the channels

- Without baseline freedom:

Fewer channels, but more concentrated and reliable → information is better attributed to the gases.

- With 1% baseline freedom:

Much higher number of channels, but with redundancy and dilution of the real information (baseline compensation).

- Indicates where to find information — by molecule and by bandwidth (LB)

CO_2		
Bands	Number of channels with 90% information	Number of channels with 90% information (Baseline fit = 0.01)
Band 1	48	170
Band 2	73	177
Band 3	69	165
Band 4	48	162
Bands 2 & 3	145	370
CH_4		
Band CH_4	42	394

Conclusion

- Coupling bands 2 & 3 for CO_2 confirms the PROFFAST choice (Detector 1).
- The PROFFAST choice for CH_4 is also validated (Detector 1).
- With Detector 2, an additional degree of information is obtained for both CO_2 and CH_4.
- The selected H_2O band (Detector 1) matches PROFFAST → choice confirmed.
- CO shows very poor sensitivity (DOFS ≈ 0.37), not usable.
- N_2O provides non-negligible information (DOFS ≈ 0.9), rarely explored.
- The covariance matrix reduces DOFS but removes redundancy and introduces vertical correlations.
- Without baseline freedom: fewer but more reliable channels. With 1% baseline freedom: more channels but redundancy and dilution.

Perspectives

- Extend H_2O analysis (two detectors, multiple bands).
- Explore the potential of N_2O retrievals.
- Automate ARAHMIS for daily full-spectrum inversions and compare outputs with PROFFAST.

Thank you for your attention