4A Direct and Inverse Radiative Transfer for Preparation and Exploitation of GHG Sounding Missions

Olivier LEZEAUX[1], Emilien BERNARD[1], Sandrine BIJAC[1], François-Marie BREON[2], Jérôme BUREAU[3], Claude CAMY-PEYRET[4], Julien CHIMOT[7], Carole DENIEL[5], Adrien DESCHAMPS[6], Emmanuel DUFOUR[1], Denis JOUGLET[6], Sébastien PAYAN[3], Clémence PIERANGELO[6], Pascal PRUNET[1], Bernard TOURNIER[1]

[1] NOVELTIS, 153, rue du Lac, F-31670 Labège, France – 4AOP@noveltis.fr –
[2] Laboratoire des Sciences du Climat et de l'Environnement (LSCE), Gif-sur-Yvette, France
[3] Laboratoire Atmosphères, Milieux, Observations Spatiales (LATMOS), Paris, France
[4] Institut Pierre-Simon Laplace (IPSL), Paris, France
[5] Centre National d'Etudes Spatiales (CNES), Paris, France
[6] Centre National d'Etudes Spatiales (CNES), Toulouse, France
[7] Now at Delft University of Technology, Delft, The Netherlands

Corresponding author: olivier.lezeaux@noveltis.fr

Summary

In the frame of the preparation and the exploitation of GreenHouse Gases monitoring missions such as MicroCarb and GOSAT, NOVELTIS was involved in many studies in which the 4A/OP code has been used for direct and inverse radiative transfer.

Thanks to CNES support, to many collaborations with scientific laboratories (CNES, IPSL, LATMOS, LSCE), and also based on own investments, NOVELTIS has developed many tools and acquired expertise for direct and inverse radiative transfer in the different infrared spectral domains (TIR, SWIR, NIR).

This poster presents the main studies and dedicated tools (listed here on the right), related to the preparation of the Microcarb Mission and the exploitation of GOSAT data, with the objective of retrieving atmospheric CO_2 product from infrared (SWIR, NIR and TIR) measurements with a correct treatment of scattering by aerosols and polarization effects.

NOVELTIS is also contributing to the preparation of European CarbonSat and Sentinel 5 missions and prepares the exploitation of OCO-2 data.

Tools available at NOVELTIS

- 4A/OP radiative transfer code (TIR,SWIR,NIR)
  - Coupled with Vlidort, Lidort, Disort scattering codes
  - SWIR/NIR Fast scattering mode
- On-going Extension of 4A/OP to UV-VIS spectral domain
- 1D-Var retrieval code with Levenberg-Marquardt iterative scheme
- Spectral Calibration tool
- Tanso-FTS polarization model

Main Studies and Applications

- Support of MicroCarb Mission
  - MicroCarb L2 Performance Orbital Simulator
  - 4ARTIC validation with 1D-Var reference tool
  - Development of Fast scattering computation
- Aerosol and cloud scattering
  - Methodologies for CO_2 retrieval with aerosol scattering
  - Aerosol Scattering Parameter retrieval from NIR/SWIR polarized measurements
  - Polarisation study from TIR Measurements
- Greenhouse Gases Retrievals
  - CO_2 retrievals from GOSAT TANSO-FTS data
  - Spectral calibration of GOSAT TANSO-FTS data
  - GOSAT Polarisation model

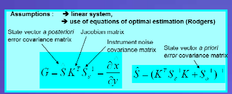
Studies using 4A and 1D-Var tools
Studies focused on signal polarisation analysis
Studies dedicated to specific tool developments

APPLICATIONS & STUDIES DESCRIPTION

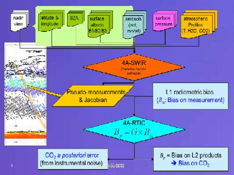
Support of MicroCarb Mission

MicroCarb L2 performance orbital simulator [1]

- Study team
  - Sandrine BIJAC (NOVELTIS),
  - Clémence PIERANGELO, Denis JOUGLET (CNES)
  - François-Marie BREON (LSCE)
- Objectives
  - MicroCarb mission goals: focus on CO_2 total net fluxes at global scale: high precision for single CO_2 measurement (1ppm) ; no regional CO_2 biases : systematic errors should not exhibit spatial structures with a typical scale of 1000 km.
  - Implementation of a « L2 performances orbital simulator » to evaluate the CO_2 spatial structure scale.
- Principle
  - Assumption that the L1 => L2 problem is linear
  - Use of Optimal Estimation formalism to compute the transport through the gain matrix of a bias on the measurement as a bias on L2 products.
  - Pseudo measurements and Jacobians are simulated with the 4A-SWIR radiative transfer model.
  - Bias transport on CO_2 L2 product is performed by means of the 4ARTIC [10] software and study of the bias spatial pattern.
- Results
  - Assessment of specific instrumental bias (8m) as a radiometric default (offset, bias taking into account the instrumental warming as a function of the position on the orbit).
  - Provide a description of realistic L2 CO_2 bias to the mission CO_2 simulator (NOVELTIS/LSCE/CNES) in order to evaluate the impact on the surface fluxes biases.



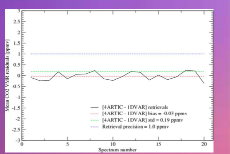
Computation of Gain matrix from instrument noise and state vector error covariance matrices and the Jacobian matrix.



Flowchart of the L2 performances orbital simulator using as input a complete and coherent geophysical database.

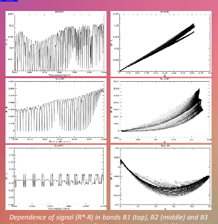
4ARTIC validation with 1D-Var reference tool [2]

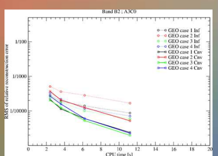
- Study team :
  - Olivier LEZEAUX (NOVELTIS),
  - Clémence PIERANGELO, Denis JOUGLET (CNES)
  - Claude CAMY-PEYRET (IPSL)
  - François-Marie BREON (LSCE)
- Context & objectives
  - For the MicroCarb mission, CNES developed a retrieval tool « 4ARTIC » (based on 4A/OP-SWIR) to provide a CO_2 product from MicroCarb measurements.
  - 4ARTIC is based on the Optimal Estimation Method developed by C.D. Rodgers [11].
  - Validation of the 4ARTIC code on specific test cases by means of the NOVELTIS retrieval code « 1D-Var » used as reference.
- Study description
  - 35 test cases with 5 scattering configurations and 7 geophysical conditions
  - Detailed analysis on one reference test case
  - Statistical analysis on the whole set of test cases
- Results
  - Retrieval precision is around 1 ppmv
  - For the reference test case, bias between 4ARTIC and 1D-Var is 0,03 ppmv and standard deviation is equal to 0,19 ppmv.
  - For the whole test cases, bias is about -0,07 ppmv and standard deviation is equal to 0,33 ppmv
- Optimal Estimation Method
  - Minimisation of the cost function : use a priori information
    $$\chi 2 = [y - f(x)]R^{-1}[y - f(x)]^T + [x - x_0]B^{-1}[x - x_0]^T$$
  - Linearization of the radiative transfer model:
    $$y = f(x) = f(x_0) + H(x_0)[x - x_0] \text{ avec } H(x_0) = \frac{\partial f}{\partial x}(x_0)$$
  - Gain matrix:
    $$G = [H^T R^{-1} H + B^{-1}]^{-1} H^T R^{-1}$$
  - Retrieval: linear solution
    $$\hat{x} = x_0 + G(x_0)[y - f(x_0)]$$


Differences between results of 4A-RTIC retrieval code and 1D-Var reference code for inversion of 20 noisy spectra.

Development of Fast scattering computation [3]

- Study team :
  - Olivier LEZEAUX (NOVELTIS),
  - Clémence PIERANGELO, Denis JOUGLET (CNES)
- Objectives :
  - Specification, development and validation of a fast scattering mode for the 4A RT code.
- Methodology
  - Classification of spectral scattering signal => channel selection
  - Exact computation of the scattering on the channel selection
  - Reconstruction of the complete spectrum with Taylor development:
  - R^* = Reflectance with scattering, R = reflectance without scattering, ν = wave number
- Analysis of reflectance scattering signal
  - Study on B1, B2 and B3 spectral bands of MicroCarb
  - Dependence of $(R^* - R) = f(R, \nu)$
    - Linear to R in B3 and quadratic to R in B1 & B2
    - Linear to ν in B2 & B3 and quasi linear in B1
- Computing time performances
  - Depends on number of classes
    - 2,5 to 19 s according to spectral band (B1,B2,B3) and number of classes (50 to 400)
    - 6,5 s in B2 and 10s in B1 with 200 classes => gain ≈ x60
- Reconstruction performances (200 classes, reference atmosphere)
  - Cirrus case (AOT=0,3) : Errors = 0,7‰ (B1), 0,3‰ (B2), 5‰ (B3)
  - Continental pollution (AOT=0,5) : Errors = 0,2‰ (B1), 0,1‰ (B2), 0,2‰ (B3)


Dependence of signal (R*-R) in bands B1 (top), B2 (middle) and B3 (bottom) as a function of the wave number (left) and the reflectance without scattering (right).


RMS of relative reconstruction error as a function of CPU time, geophysical scenario. Case of cirrus in band B2 for high resolution spectrum (inf) and convolved spectrum with B2 ISRF (Cnv).

Aerosol and cloud scattering

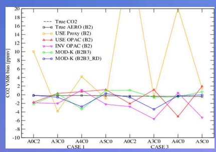
Methodologies for CO2 retrieval with Aerosol scattering [4]

- Study team
  - Olivier LEZEAUX (NOVELTIS),
  - Clémence PIERANGELO, Denis JOUGLET, Adrien DESCHAMPS (CNES)
  - Claude CAMY-PEYRET (IPSL)
  - François-Marie BREON (LSCE)
- Objectives
  - CO_2 retrieval method analysis in presence of aerosols
  - Specification of CO_2 retrieval methodology for the 4ARTIC code
- CO_2 retrieval
  - Use only B2 for Proxy and OPACs methods
  - Use B2 and B3 for k-model methods

Name	Description	Solar Zenithal Angle	Albedo	P_{surf}	Atmosphere
Case 1	référence	30°	Vegetation	standard	Hot / weat
Case 2	Impact angle solaire	60°	Vegetation	standard	Hot / weat
Case 3	Impact albédo fort	30°	Desert	standard	Hot / weat
Case 4	Impact albédo faible	30°	Dark surface	standard	Hot / weat

Name	Description	Altitude	AOT at 0.55 µm	AOT at 0.75 µm	AOT at 1.6 µm
A0C2	High altitude cirrus	15km	0.4	0.40	0.41
A3C0	Continental polluted mixture	1-3 km	0.5	0.32	0.09
A4C0	Desert dust mixture	4-6 km	0.5	0.29	0.26
A5C0	Tropical oceanic mixture	0-1 km	0.5	0.30	0.25
A3C2	Continental polluted + Cirrus	1-3 km et 15 km	0.9	0.72	0.50

Description of geophysical scenarios and aerosol types.

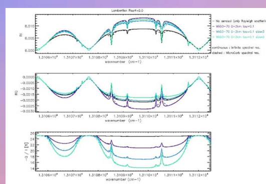


Bias on CO_2 VMR retrieval according to the geophysical case, the aerosol type and the methodology used. B2B3_RD stands for reduced intervals of 10 cm^{-1} for both spectral bands.

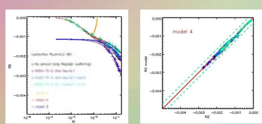
- Aerosol retrieval methodologies
  - Proxy : Ps retrieval on B1 and B2, CO_2 retrieval on B2
    $$\text{Proxy}: CO_2 = CO_2(B2)\frac{P_S(B1)}{P_S(B2)}$$
  - USE-OPAC : B1 Autotyped retrieval then transport to B2 with OPAC model
  - INV-OPAC : B1 AOT+type retrieval then B2 AOT retrieval with OPAC model
  - MOD-K : B1 AOT+altitude retrieval then B2/B3 k retrieval with k-model
    $$\text{k-model}: AOT(\nu) = AOT(\nu_0)\left[\frac{\nu}{\nu_0}\right]^k$$
- Results
  - Proxy method not appropriate
  - Better results with k-model than OPAC, especially for case 3
  - Mean bias around -0,5 ppmv
  - Standard deviation ~1,5 ppmv

Aerosol Scattering Parameters retrieval from NIR/SWIR polarized measurements [5]

- Study team :
  - Emmanuel DUFOUR, Emilien BERNARD (NOVELTIS),
  - Clémence PIERANGELO (CNES)
  - François-Marie BREON (LSCE)
- Objectives
  - Exploitation of the polarization information contained in NIR/SWIR high resolution spectra in order to improve characterization of aerosols and cirrus.
- Methodology
  - Analysing polarization information contained in the I and Q Stokes components of the incoming signal
    - O_2-A absorption band (around 0.75 µm)
    - SWIR CO_2 absorption bands (~1.61 µm and 2.0 µm)
  - High spectral resolution polarised radiative transfer simulations for around 50 different atmospheric (aerosol, cirrus) and surface (Lambertian, ocean glint) scenario.
  - Development of an aerosol retrieval method based on a Look Up Table retrieval scheme relying on the regressed form of the considered radiative transfer simulations.
- Results
  - According to the MicroCarb mission characteristics, aerosol retrieval scores of more than 75% are found for the majority of the atmospheric scenarii.
  - Analogous retrieval tests in the presence of perturbed CO_2 concentration demonstrate the high potential of the method for separating the CO2 signal from the aerosol signal.
  - The next step will be to quantify the benefit of the proposed approach on real data using GOSAT polarized measurements.
- Acknowledgments
  - Laurent Labonnote (LOA)
  - Robert J. D. Spurr (RT Solutions, Inc.)



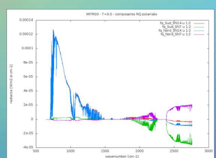
Impact due to different sizes of an aerosol OPAC WASO 70, for nadir view and 40° solar zenithal angle, and surface reflectance equal to zero. From top to bottom: RI, RQ and polarisation factor –Q/I.



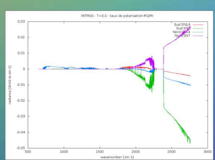
Left : RQ_model = f(RI) with models 1, 3 et 4 overlaying the simulated signals (RI, RQ). Profiles WASO-70 with size variation for the Lambertian scenario. Right : RQ_model vs. RQ observed in MicroCarb B1 spectral band for the different models compared to radiometric noise at ±1 sigma for the considerate case (dashed lines).

Polarisation study from TIR Measurements [6]

- Study team :
  - Sandrine BIJAC, Emmanuel DUFOUR, Bernard TOURNIER (NOVELTIS),
  - Adrien DESCHAMPS (CNES)
- Objectives
  - Analysis of atmospheric signal polarisation of TIR IASI-NG measurements
    - Realistic aerosol distributions set up
    - Sensitivity study of IASI-NG spectra according to aerosol distribution polarisations
- Tools
  - 4AOP-Subroutine SWIR/TIR (release-72-subroutine-27) + VLIDORT 2P5



Polarised component RQ of IASI-NG spectra in the case of MITR aerosol with AOT of 3.0, for daytime nadir and high angle views in tropical area (lat=+/-20°).



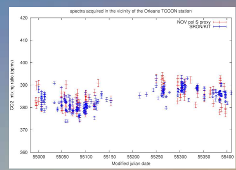
Polarisation factor RQ/RI of IASI-NG spectra in the case of MITR aerosol with AOT of 3.0, for daytime nadir and high angle views in tropical area (lat=+/-20°).

- Main results
  - The polarisation factor is very small (< 1%) in TIR region
  - The polarisation factor is significant in MWIR solar region for MITR type aerosol
  - The polarisation factor is maximal at nadir view

Greenhouse Gases Retrievals

CO2 retrievals from GOSAT TANSO-FTS data [7]

- Study team
  - Olivier LEZEAUX, Julien CHIMOT (NOVELTIS)
  - Carole DENIEL, Clémence PIERANGELO (CNES)
  - Claude CAMY-PEYRET (IPSL)
  - François-Marie BREON (LSCE)
  - Jérôme BUREAU, Sébastien PAYAN (LATMOS)
- Objectives
  - Atmospheric CO_2 retrievals from NIR-SWIR GOSAT TANSO-FTS spectra over 6 TCCON stations and Solar Village site.
  - CO_2 product validation by intercomparison with TCCON products and other GOSAT CO_2 products (NIES, ACOS, SRON/KIT, U. Leicester).
- CO_2 retrieval methodology
  - Albedo (mean value + slope), surface pressure, CO_2 and H_2O total content retrievals from B2.
  - Aerosol AOT and type, albedo (mean value + slope) and surface pressure (Ps) retrievals from B1. Aerosol retrieval and proxy factor Ps(B1)/Ps(B2) are used to improve CO_2 retrieval from B2.



NOVETIS CO_2 product (blue) and SRON/KIT CO_2 product (red) obtained from GOSAT TANSO-FTS spectra over Orléans TCCON station.

Differences of the retrieved XCO_2 (5 algorithms) with respect to TCCON (all in ppm)

nb= number of coincident retrievals (IFOVs in the vicinity of TCCON stations the same day)
bias=mean(retrieval – TCCON) for S spectra
stdv=standard deviation around the mean

Orléans
```
Leicester - TCCON nb=  7 bias=-0.89 stdv=1.94
SRON/KIT  - TCCON nb= 25 bias=-1.63 stdv=1.72
NIES(L2)  - TCCON nb=  9 bias=-1.86 stdv=1.64
NOV       - TCCON nb= 14 bias=-2.54 stdv=2.55
ACOS B2.9 - TCCON nb= 14 bias= 0.17 stdv=1.50
```
Lamont
```
Leicester - TCCON nb= 27 bias=-1.48 stdv=3.77
SRON/KIT  - TCCON nb= 96 bias=-0.75 stdv=1.64
NIES(L2)  - TCCON nb= 28 bias=-2.41 stdv=1.21
NOV       - TCCON nb= 44 bias=-1.06 stdv=2.71
ACOS B2.9 - TCCON nb= 26 bias=-1.22 stdv=2.04
```
Darwin
```
Leicester - TCCON nb= 18 bias=-0.97 stdv=2.70
SRON/KIT  - TCCON nb= 20 bias=-1.13 stdv=1.52
NIES(L2)  - TCCON nb= 10 bias=-2.94 stdv=0.93
NOV       - TCCON nb= 11 bias= 0.89 stdv=2.60
ACOS B2.9 - TCCON nb= 13 bias=-1.19 stdv=0.68
```
Negative bias for (almost) all GOSAT retrievals with respect to TCCON

The stdv is consistent with the combined RSS of the retrieval errors and of those of TCCON data

<bias>=-1.27
<stdv>= 1.94

- Pre-Post screening criteria
  - CO2 retrievals are filtered according to diagnostic parameters
    - Pre-filtering on spectra with simple B4 cloud/aerosol detection scheme (J. Bureau /C. Camy-Peyret)
    - Nb of iterations ≤ 3
    - Error on CO2 < 2 ppmv, $\chi 2_\nu < 0.8$
    - Correction with proxy < 1 % (ΔPsurf ≤ 10 hPa)
- Intercomparison Results
  - NOVELTIS retrievals are in very good agreement with SRON/KIT
  - All retrievals are quite consistent (no bias correction applied) : <bias>=0.43 ; <stdv>=3.04
  - Negative bias for almost all GOSAT retrievals with respect to TCCON : <bias>=-1.27 ; <stdv>= 1.94

- Acknowledgments
  - JAXA and NIES for allowing access to GOSAT data
  - The ETHER data center
  - H. Bösch (Univ. of Leicester) for TANSO-FTS XCO2 retrievals
  - J. Landgraff & O. Hasekamp (SRON) and A. Butz (KIT) for TANSO-FTS XCO2 retrievals as well as data from the stations of the TCCON network
  - D. Crisp, A. Eldering and C. O'Dell for providing the ACOS L2 products

Spectral calibration of GOSAT TANSO-FTS data [8]

- Study team
  - Olivier LEZEAUX, Julien CHIMOT, Emmanuel DUFOUR (NOVELTIS)
  - Carole DENIEL (CNES)
  - Claude CAMY-PEYRET (IPSL)
  - Jérôme Bureau, Sébastien PAYAN (LATMOS)
- Objectives
  - Development and validation of a spectral calibration tool
  - Spectral calibration processing of GOSAT TANSO-FTS data
  - Provide calibrated spectra to end users
- Spectral calibration methodology
  - Specification of 2-3 intervals per spectral band
  - Compute synthetic reference spectrum with 4A-SWIR code taking into account the Doppler shift effect
  - Use mean scale factor obtained from the 2-3 intervals of each spectral band
  - Processing independent of the retrieval scheme

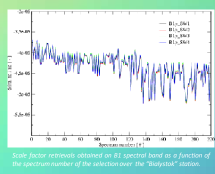
Domaine spectral de calibration	B1-2	B1-3
Bornes (en cm^{-1})	13000-13060	13060-13120

Domaine spectral de calibration	B2-1	B2-3	B2-4
Bornes (en cm^{-1})	6030-6120	6200-6260	6320-6390

Domaine spectral de calibration	B3-2	B3-3
Bornes (en cm^{-1})	4810-4850	4850-4890

Domaine spectral de calibration	B4-1	B4-5
Bornes (en cm^{-1})	730-760	1240-1300

- Acknowledgments
  - JAXA and NIES for allowing access to GOSAT data
  - The ETHER data center

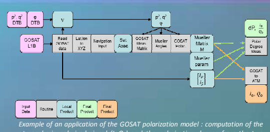


Scale factor retrievals obtained on B1 spectral band as a function of the spectrum number of the selection over the "Bialystok" station.

- Performances
  - The spectral calibration tool uses the solid expertise acquired at NOVELTIS on the IASI spectral calibration
  - This particular processing allows to provide to scientific users (via the ETHER centre) totally calibrated GOSAT spectra
  - Retrieval errors on the scale factor $\Delta\nu/\nu$ have been evaluated to 2.10^{-7} for B1 and B2 bands and $4\ 10^{-7}$ for B3 and B4 bands. The relative precision on the scale factor retrieval is then ~0.5% for B1 & B2, and ~1% for B3 & B4.
- End-user applications
  - More than 40,000 GOSAT spectrally calibrated spectra are available at the ETHER centre.
  - These calibrated spectra have been also provided to ESA in the frame of the exploitation of spectral SWIR-TIR synergy for CH_4 retrieval in the lower atmosphere.

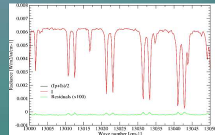
GOSAT Polarisation model [9]

- Study team
  - Olivier LEZEAUX, Sandrine BIJAC (NOVELTIS)
  - Carole DENIEL, Denis JOUGLET (CNES)
  - Claude CAMY-PEYRET (IPSL)
  - Sébastien PAYAN (LATMOS)
- Objectives
  - Development of a polarization model dedicated to GOSAT data
  - Processing of GOSAT data with correct treatment of polarized signal



Example of an application of the GOSAT polarization model : computation of the atmospheric polarized signal (I_0,Q_0) and the polarization degree from the two polarized components I_P & I_S measured by the TANSO-FTS on GOSAT.

- Polarisation model formalism
  - To compute I_P & I_S from I_0 & Q_0
  - To compute I_0 & Q_0 from I_P & I_S … or
    $$I_0 \approx \frac{I_P + I_S}{2}, \quad Q_0 \approx \frac{I_P - I_S}{2\delta}$$
- Applications
  - To compute the atmospheric polarized spectrum (total intensity I_0 and polarized component Q_0) from the polarized P and S GOSAT L1b components.
  - To simulate the I_P and I_S polarized components of GOSAT L1b spectra from an atmospheric polarized spectrum (I,Q).
  - Allows verifying the approximated formula : $I_0 = \frac{I_P + I_S}{2}$



Example of computation of the atmospheric polarized signal (I_0,Q_0) from the two polarized components I_P & I_S measured by the TANSO-FTS on GOSAT. Exact formula with the polarization model (red), approximated formula (black) and residuals (green).

- Acknowledgments
  - Many thanks to Denis O'Brien (Colorado State University) for providing the GOSAT polarisation model

Studies and efforts in progress…

- Consolidation of GOSAT processing chain for atmospheric CO_2 and CH_4 retrieval
- Adaptation of the GOSAT processing chain to OCO-2 data
- SWIR/TIR spectral synergy analysis for lowermost atmospheric GHG retrieval
- Exploitation of GHG level 2 products for deriving level 4 products : point source fluxes estimates (industrial emissions)
- Consolidation of direct/inverse tools for improving product characterisation and performance analysis : principal component decomposition, improved information content analysis and error characterisation.

Perspectives

- Exploitation of OCO-2 measurements for atmospheric CO_2 retrieval and analysis
- Application of the aerosol retrieval scheme using polarisation on GOSAT and OCO-2 measurements
- Contribution to the preparation of future missions
  - CarbonSat
  - Sentinel 5
  - Sentinel 5 / IASI-NG synergies
  - MTG-IRS
  - Other concepts of GHG sounding missions …

References

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