Potential of TIR+SWIR combination from space measurements for CH_4 retrievals: application to IASI and S5P

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Context

- Atmospheric CH_4 is measured continuously from space-borne passive optical instruments, providing valuable information at global and regional for atmospheric monitoring and for surface flux estimates.
- Instruments in the SWIR provide a total atmospheric column with rather uniform sensitivity up to the tropopause (including the lowermost layers).
  - Past and current instruments : SCIAMACHY, GOSAT TANSO-FTS, S5P TROPOMI
  - Planned : Sentinel 5 - UVNS
- Nadir instruments in the TIR provide profile information, with typically a few pieces of information in the middle and upper troposphere.
  - Past and current instruments : TES, CrIS, IASI
  - Planned : IASI-NG

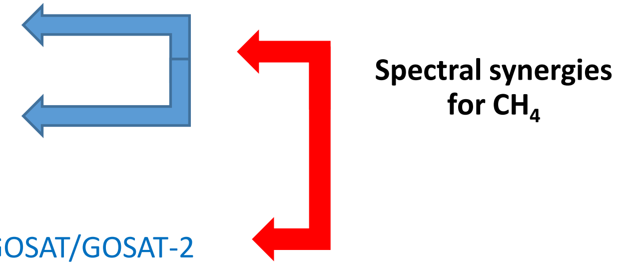
CH_4 absorption domains:

SWIR1 : 1.6 µm : S5 (1595 – 1675 nm), GOSAT /GOSAT-2

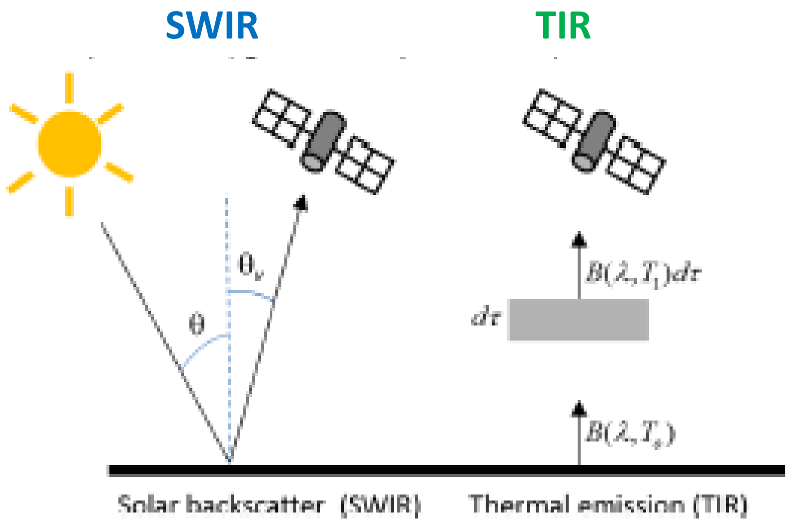
SWIR3 : 2.3 µm : S5P & S5 (2305 – 2385 nm), GOSAT-2

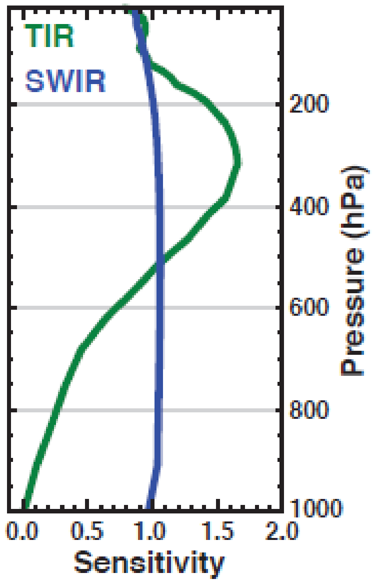
TIR (MWIR) : 3-3.7 µm (2700-3200 cm^{-1}) : ACE-FTS

TIR (LWIR) : 7-8.3 µm (1200-1400 cm^{-1}) : IASI, IASI-NG, CrIS, GOSAT/GOSAT-2



Context





Combination should give more sensitivity to the surface

CH_4 absorption domains:

SWIR1 : 1.6 µm : **S5** (1595 – 1675 nm), GOSAT /GOSAT-2

SWIR3 : 2.3 µm : **S5P** & **S5** (2305 – 2385 nm), GOSAT-2

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TIR (LWIR) : 7-8.3 µm (1200-1400 cm^{-1}) : **IASI**, **IASI-NG**, CrIS, GOSAT/GOSAT-2

Spectral synergies for CH_4

IASI-NG and S5-UVNS onboard Metop-SG

Objective and Outline

Objective :

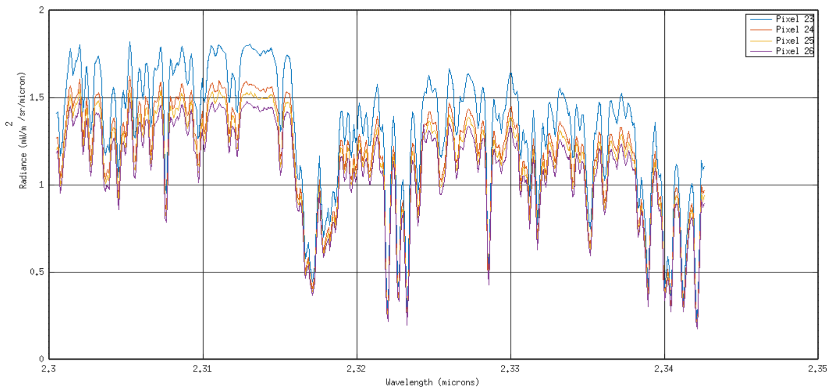
- **Defining and developing algorithms** for the joint TIR+SWIR retrieval from IASI and TROPOMI, preparing exploitation of IASI-NG and Sentinel 5 UVNS.
- **Investigate the added value of combining SWIR and TIR measurements for CH_4 retrievals** from satellite in order to obtain consolidated information on lower tropospheric methane and on vertical profile.
- **Investigate the consistency of using TROPOMI and IASI** datasets for that purpose.

Outline :

- **Theoretical analysis of SWIR+TIR synergy in different configurations** L1(TIR)+L2(SWIR) or L1(TIR)+L1(SWIR).
- **Dealing with real data** : IASI TIR retrieval of CH_4 and preparation of L1(IASI)+L2(TROPOMI)

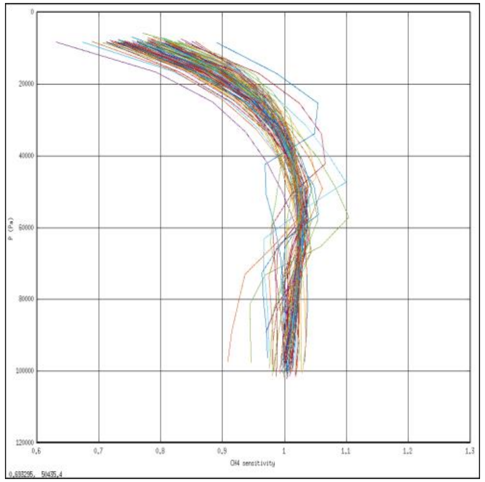
Theoretical analysis : SWIR (TROPOMI, S5P)

- **From a careful analysis of TROPOMI L1 et L2 product as a reference …**

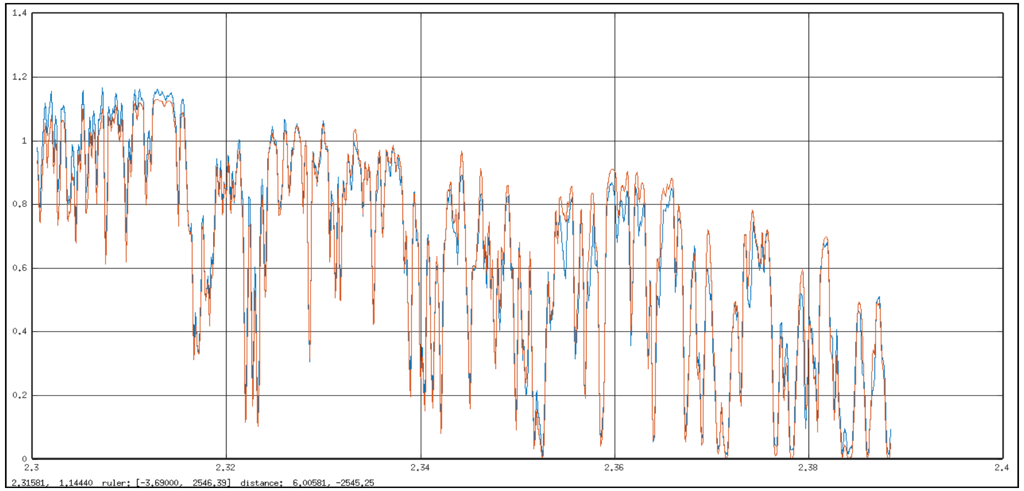


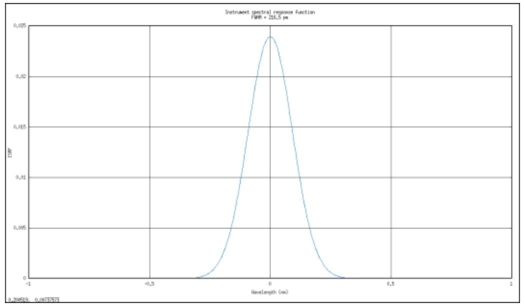
TROPOMI L1B radiances (band 7) for few pixels

Example of column averaging kernels from TROPOMI L2 CH_4 product (100 kernels randomly chosen)



- **… Simulation of idealised (but realistic) synthetic spectra/jacobian with the 4A/OP radiative transfer**





Example of TROPOMI spectrum simulated on B7 and B8, obtained from 4A/OP direct simullation with an « idealised » Gaussian ISRF

4A/OP also provides Jacobians, and we compute synthetic AK and retrieval uncertainty from Optimal Estimation formalism

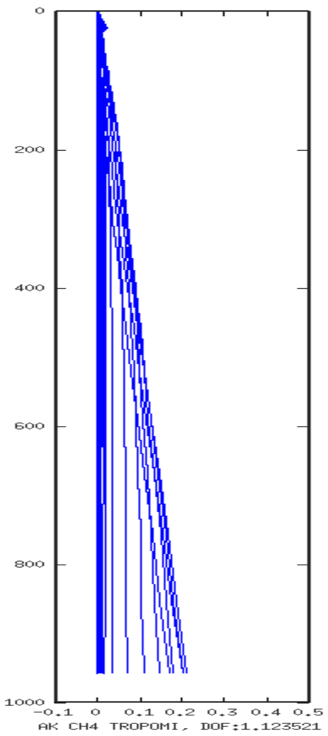
Theoretical analysis : SWIR (TROPOMI, S5P)

Information content analysis : Averaging Kernels, Degree Of Freedom For Signal (DOFS)

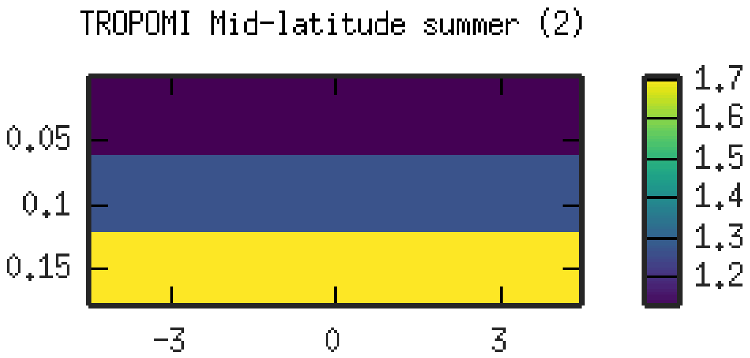
OEM analysis in different conditions (atmosphere, surface thermal contrast, albedo, surface pressure, observation and solal zenith angles) and with different hypotheses on CH_4 *a priori* constraint.

Atm	ΔT	albedo	P	OZA	SZA	DOFS	σXCH_4 posterior (ppb)
Mid Lat Summer	0.0	0.03	1013	30	30	1.12	5.51

TROPOMI averaging kernels



TROPOMI DOFS as a function of albedo (lines) and thermal contrast (colimns)



Tropical

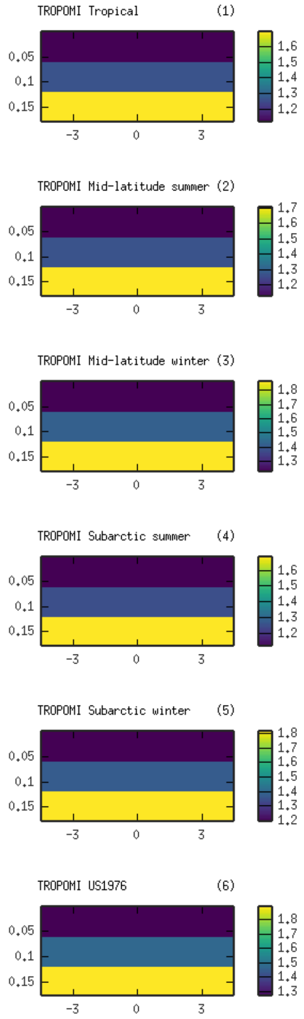
Mid Lat Summer

Mid Lat Winter

Sub Arctic Summer

Sub Arctic Winter

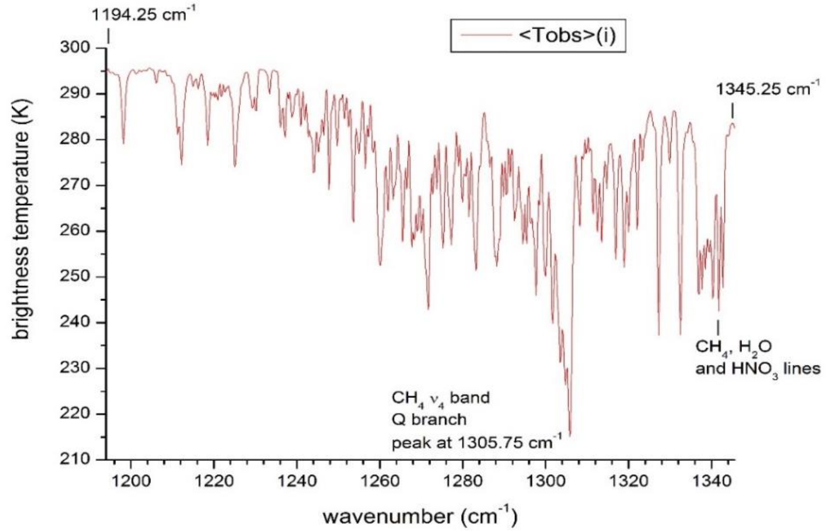
US Standard



TROPOMI DOFS as a function of atmospheres

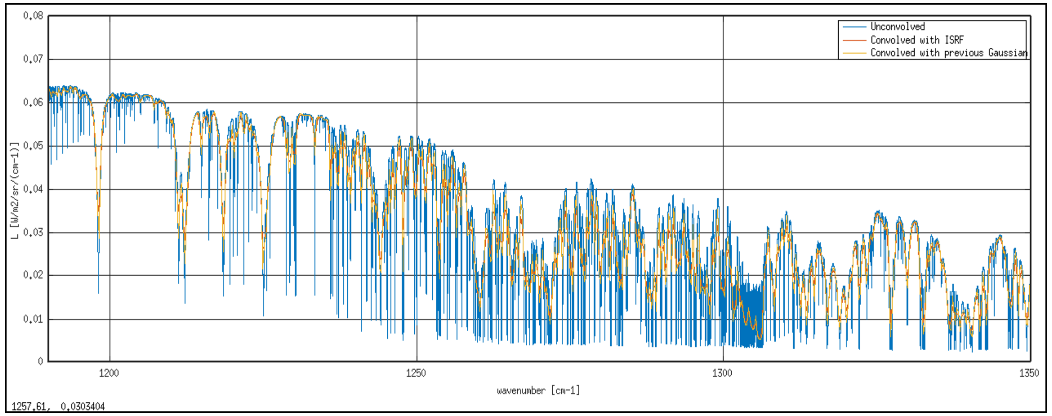
Theoretical analysis : TIR (IASI)

- **Optimised choice of a dedicated spectral domain : [1190 - 1350 cm^{-1}]** **(based on ESA CH4TIR study, see Charles Robert talk)**



- Line-mixing effects dominate in the right wing of the Q branch around ~ 1305-1309 cm^{-1}
- Complicated region at ~ 1337-1342 cm^{-1} : overlapping of CH_4, H_2O and HNO_3 lines : possible misfit for H_2O and HDO lines : inconsistency of H_2O and HDO spectroscopy; possible effect of CH_4 line-mixing
- The specific dependence of the absorption on the right side of the Q branch will be beneficial (provided that the LM model is well "calibrated") for probing the lower layers where the effect of pressure are highest at 1307.25 cm^{-1}
- The least absorbed (highest BT) spectral samples around 1285.25 cm^{-1} and 1315.75 cm^{-1} will be constraining CH_4 in the lowest levels/layers with less constrain on T_{surf} and emissivity but these micro-windows will be good for these latter parameters if LM is properly accounted for in the forward model

- **Simulation of spectra and Jacobians with 4A/OP:**



Example of IASI spectrum simulated with 4A/OP.

Jacobians are also provided, and we compute synthetic AK and retrieval uncertainty from Optimal Estimation formalism

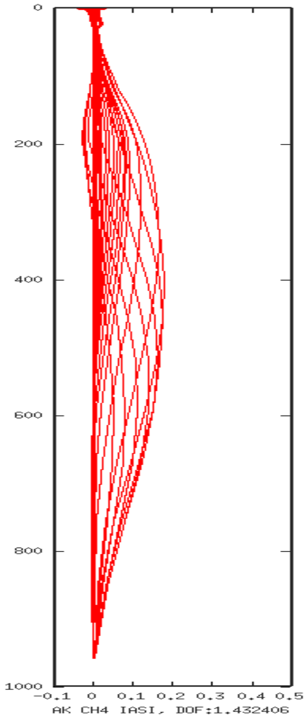
Theoretical analysis : TIR (IASI)

Information content analysis : Averaging Kernels, Degree Of Freedom For Signal (DOFS)

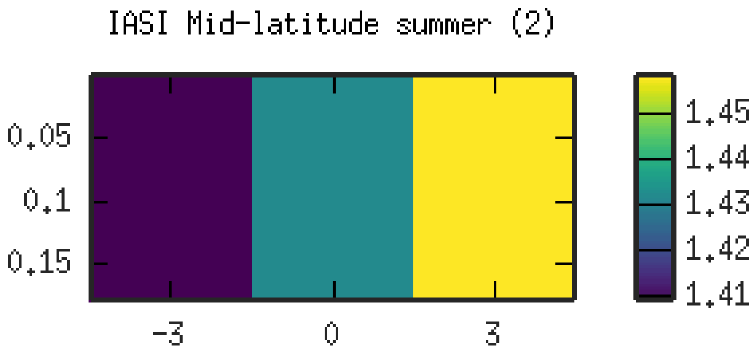
OEM analysis in different conditions (atmosphere, surface thermal contrast, albedo, surface pressure, observation and solal zenith angles) and with different hypotheses on CH_4 *a priori* constraint.

Atm	ΔT	albedo	P	OZA	SZA	DOFS	σXCH_4 posterior (ppb)
Mid Lat Summer	0.0	0.03	1013	30	30	1.43	26.67

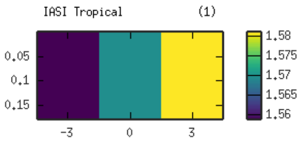
IASI averaging kernels



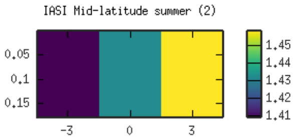
IASI DOFS as a function of albedo (lines) and thermal contrast (colimns)



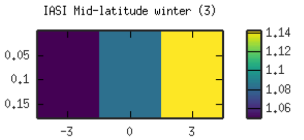
Tropical



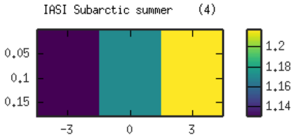
Mid Lat Summer



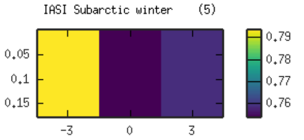
Mid Lat Winter



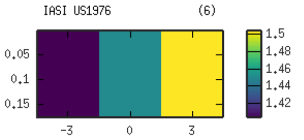
Sub Arctic Summer



Sub Arctic Winter



US Standard



IASI DOFS as a function of atmospheres

Theoretical analysis : TIR + SWIR combinations

- **Tested configurations for SWIR and TIR CH_4 retrieval:**

  - **L1(IASI)** TIR only inversion of IASI spectrum
  - **L1(TROPOMI)** SWIR only inversion of TROPOMI spectrum
  - **L1(IASI)+L1(TROPOMI)** combined (SWIR+TIR) inversion of IASI spectrum and TROPOMI spectrum
  - L2(TROPOMI) vertical integration of CH_4 profile retrieved from the SWIR inversion of TROPOMI spectrum
  - P2(TROPOMI) vertical profile of CH_4 retrieved from the SWIR inversion of TROPOMI spectrum (retrieved on 39 layers)
  - **L1(IASI) + L2(TROPOMI)** combined (SWIR+TIR) inversion of IASI spectrum and TL2(TROPOMI) product
  - **L1(IASI) + P2(TROPOMI)** combined (SWIR+TIR) inversion of IASI spectrum and P2(TROPOMI) product

All inversion configurations use 4A/OP and the OEM formalism to retrieve a CH_4 profile on 39 layers

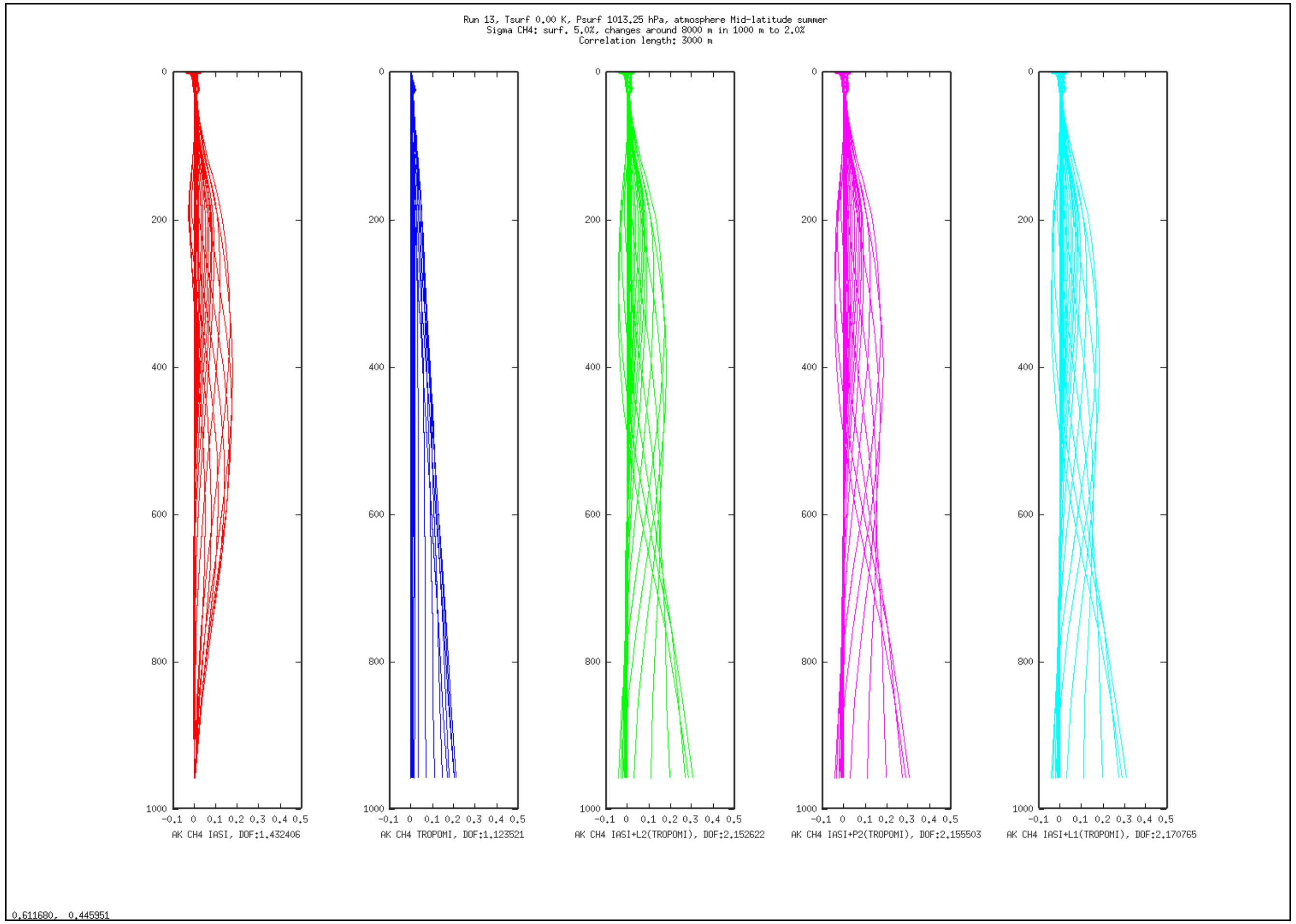
Theoretical analysis : TIR + SWIR combinations

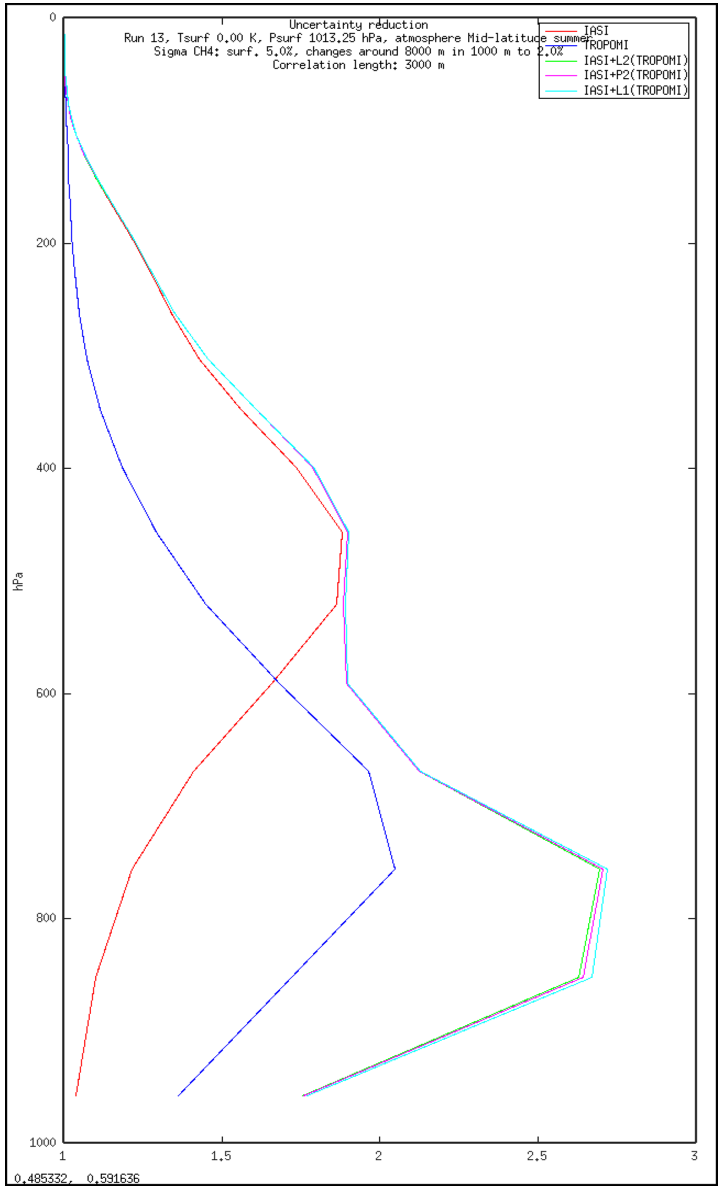
- **Results in terms of DOFS and retrieval uncertainty on the column, for mid latitude summer atmosphere:**
  - Extensive tests (uncertainty transport and iterative retrieval from synthetic data):
    - 54 scenarios for 6 atmospheres, with different values for thermal contrast (-3 K, 0 K et +3 K) and albedo (0.03, 0.05 et 0.15).
    - DOFS IASI between 0.75 and 1.5, DOFS TROPOMI between 1.1 and 1.8, IASI+L2(TROPOMI) between 1.6 and 2.3.
  - Larger impact of the synergy obtained with low albedos

Sim	Atm (km)	ΔT (K)	albedo	P (hPa)	OZA(°) IASI	OZA(°) S5P	SZA(°) S5P	DOFS IASI	DOFS S5P	L1(IASI)+ L2(S5P)	L1(IASI)+ P2(S5P)	L1(IASI)+ L1(S5P)	σXCH_4 (ppb) posterior IASI,S5P, L2,P2,L1
10	2	-3.0	0.03	1013	30	30	30	1.409	1.123	2.155	2.157	2.173	27.48 5.51 5.42 5.35 5.26
13	2	0.0	0.03	1013	30	30	30	1.432	1.124	2.153	2.156	2.171	26.67 5.51 5.42 5.34 5.25
16	2	3.0	0.03	1013	30	30	30	1.458	1.124	2.151	2.154	2.169	25.81 5.51 5.41 5.33 5.24

Theoretical analysis : TIR + SWIR combinations

- Results in terms of averaging kernels (right) and uncertainty reduction on CH_4 profile (left), for mid latitude summer atmosphere, no thermal contrast, low albedo:





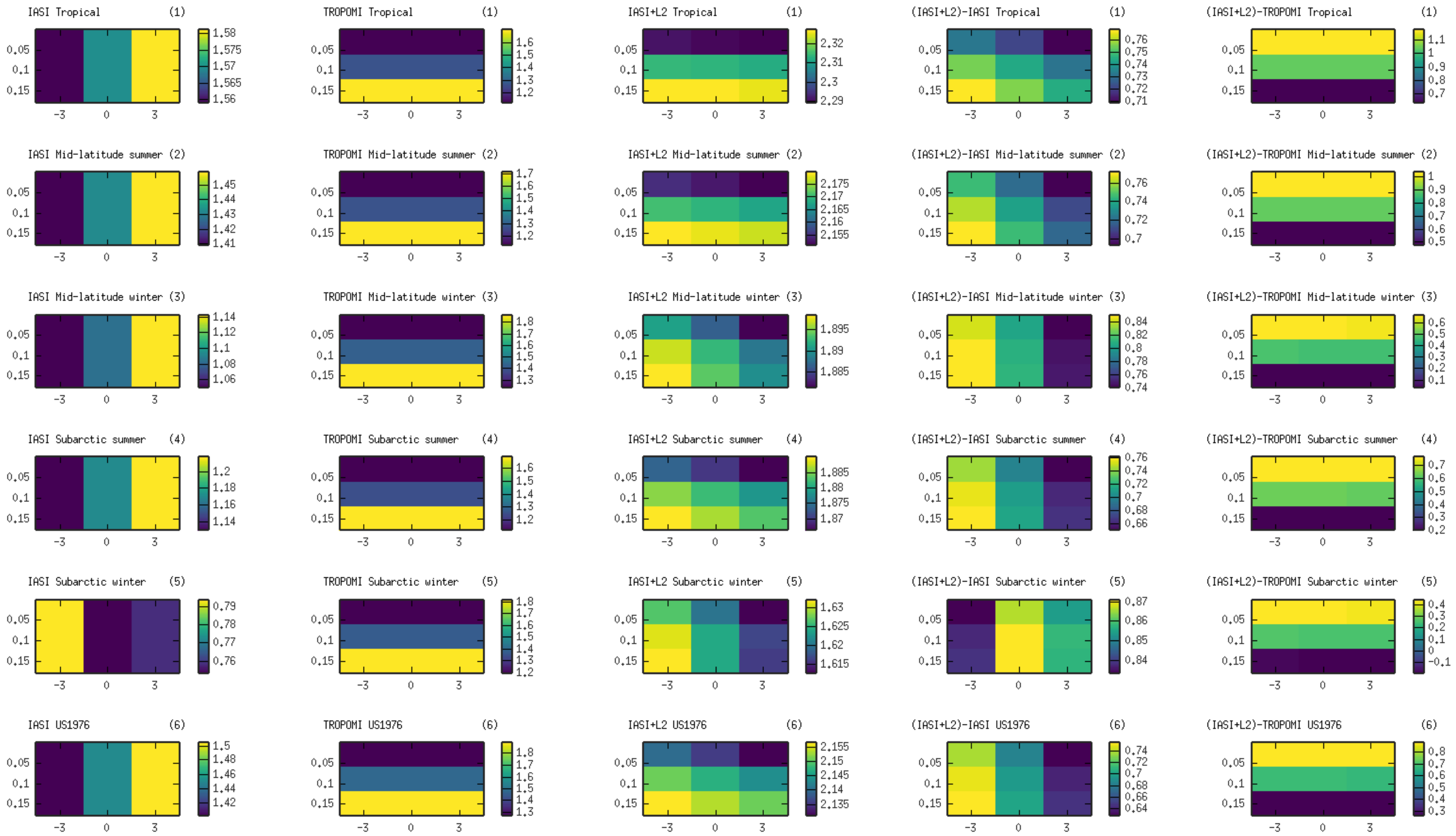
Theoretical analysis : TIR + SWIR combinations

- DOFS variations as a function of 54 scenarios (atmosphere, thermal contrast, albedo) and instrument configurations

Additional DOFS due to synergy varies between 0 and 1, most of the time above 0.5.

With respect to TROPOMI alone, largest added value of IASI is mostly for low albedos.

With respect to IASI alone, more complex figures. Synergy seems to be favourable in case of negative thermal contrast, but depends on the atmosphere. The additional DOFS is most of the time above 0.7



Algorithm implementation for application to real data

- **OEM formalism for L1(IASI) + L2(TROPOMI), with 4A/OP forward model: cost function**

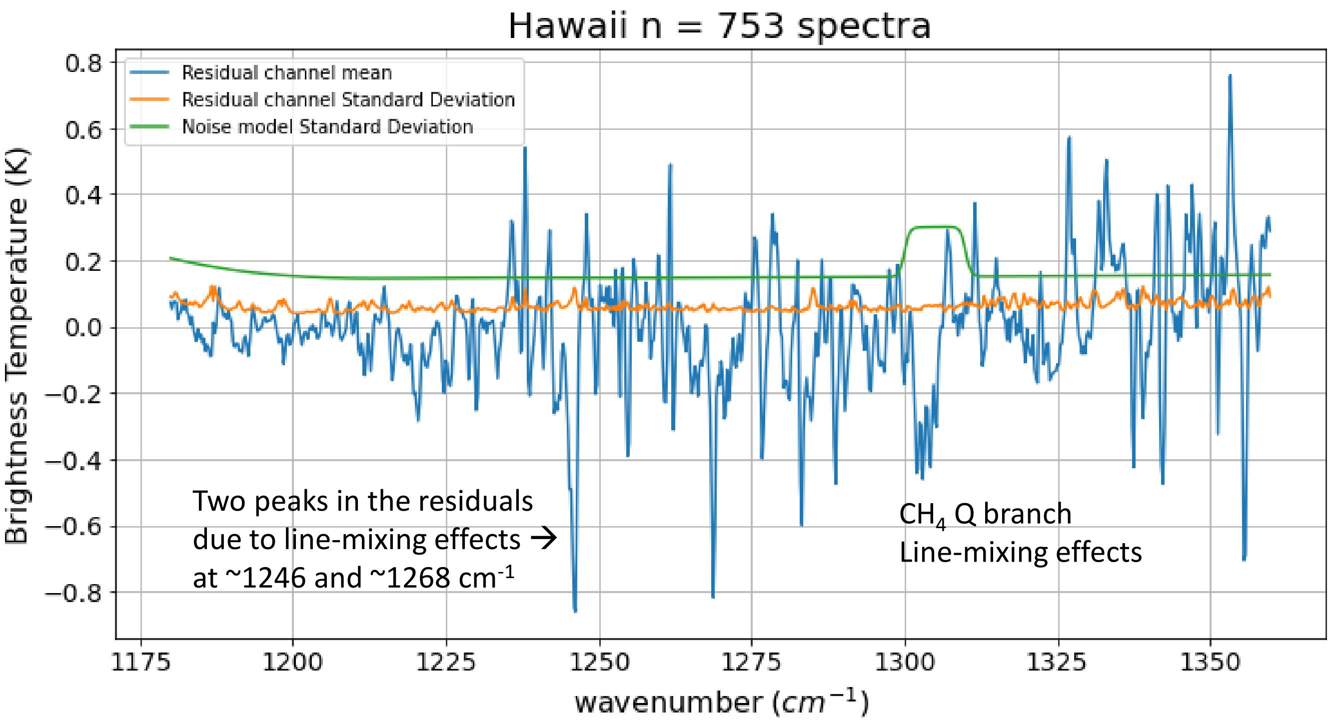
$$\chi^2 = (\mathbf{y} - \mathbf{f}(\mathbf{x},\mathbf{b}))^T \mathbf{S_y}^{-1}(\mathbf{y}-\mathbf{f}(\mathbf{x},\mathbf{b})) + (Y - F(\mathbf{x},\mathbf{b},\mathbf{b'},\mathbf{x_a'})) S_Y^{-1} (Y - F(\mathbf{x},\mathbf{b},\mathbf{b'},\mathbf{x_a'})) + (\mathbf{x}-\mathbf{x_a})^T\mathbf{S_x}^{-1}(\mathbf{x}-\mathbf{x_a})$$

(Back up slide for details and discussion)

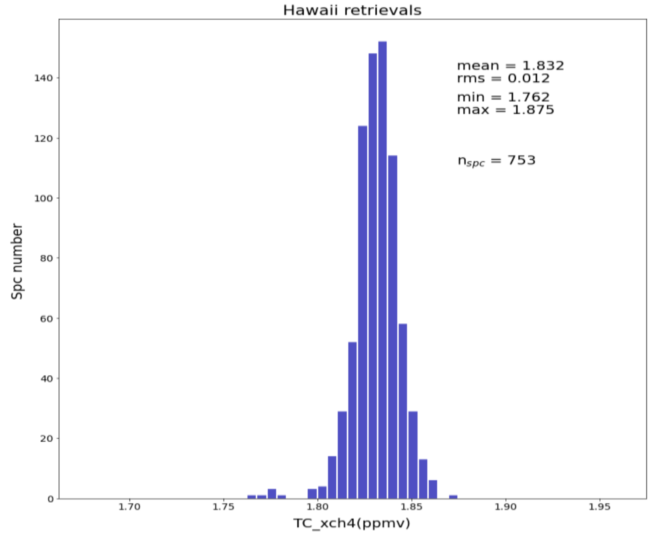
Algorithm implementation for application to real data

- **First tests on L1(IASI) only :** the objective was to validate the algorithm using 4A/OP as forward model
- **Retrievals from IASI L1C over Hawaii, January 2016 (test dataset extensively used for validation and intercomparison of UniBas, BIRA and SPASCIA algorithms)**

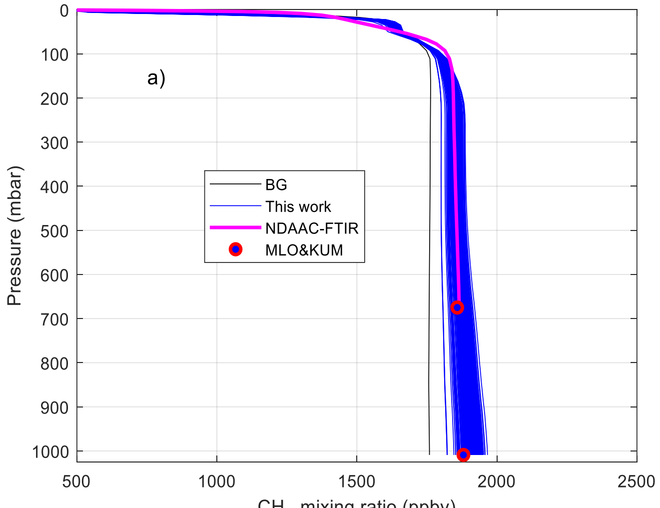
Mean spectral residuals from retrieved state (obs – calc)



Extensive discussion of residuals in Charles Robert (BIRA) talk



XCH_4 retrievals

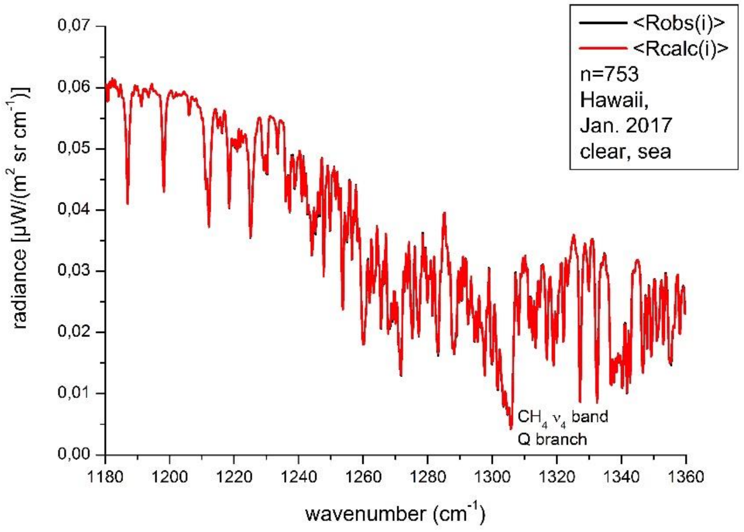


CH_4 profile retrievals compared with reference data

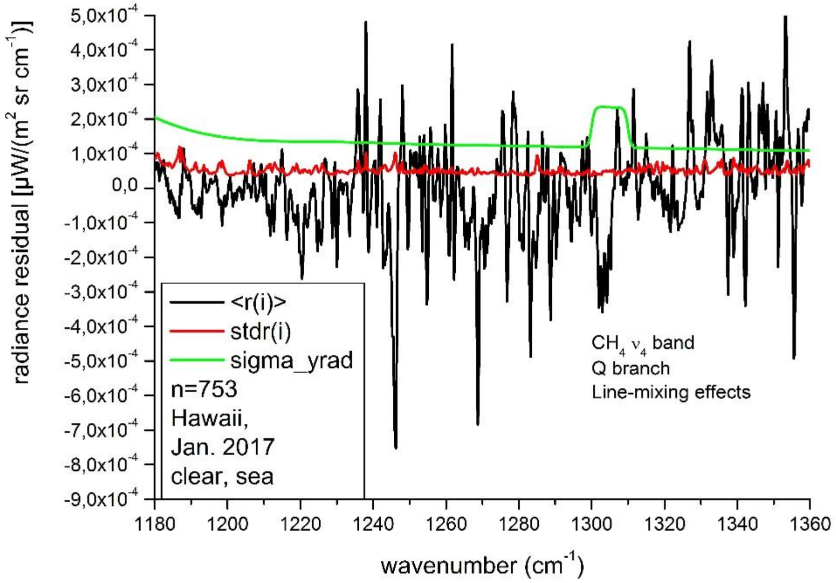
Hawaii retrievals on L1(IASI)

- **In figure on the left, over the full CH_4 retrieval domain, the spectra R_{obs} and R_{calc} show barely any difference. Overall, at this scale the retrieval is satisfactory**
- **The differences are better seen in the residuals of figure on the right. The largest residuals are around the Q branch at 1306 cm^{-1} where LM effects are important. But because of the use of an inflation factor, this region has a reduced weight in the retrieval (green curve)**

Mean spectral from retrieved state (Robs, Rcalc)



Mean spectral residuals from retrieved state (obs – calc)

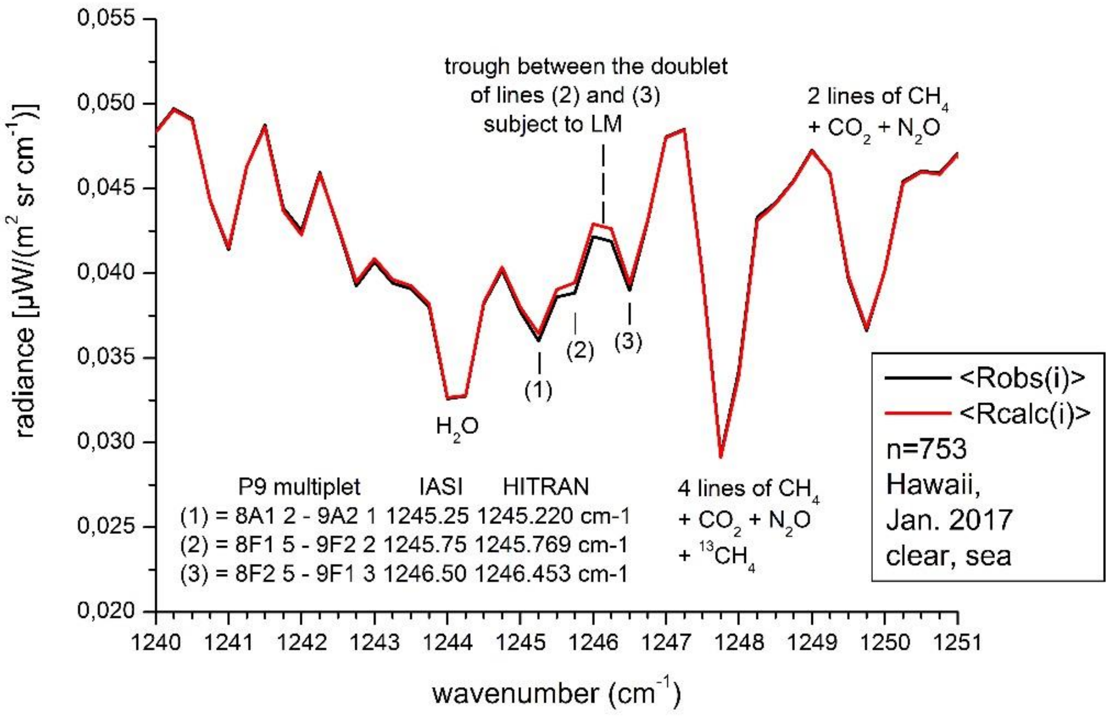


Hawaii retrievals on L1(IASI)

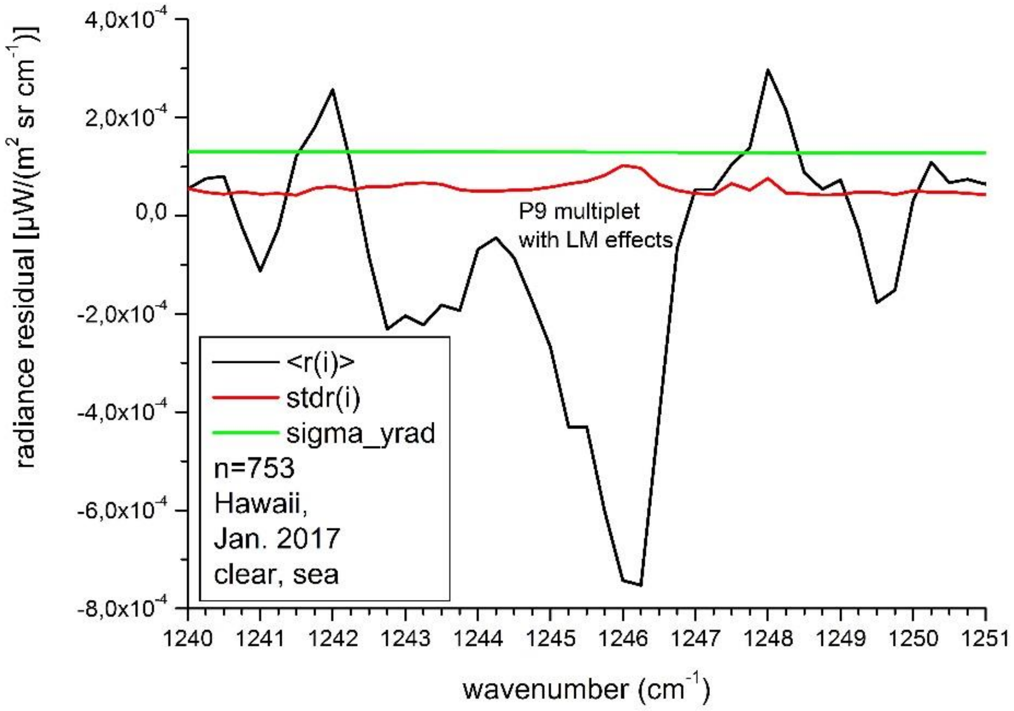
- **The following figures provide zooms in specific regions where peaks in the residuals are seen :**
  1246 cm^{-1} → P9 multiplet (this slide) and 1268 cm^{-1} → P6 multiplet (next slide)
- **These two regions in the P branch of the ν_4 band of CH_4 show line-mixing effects in the P9 and P6 multiplets : Incomplete modelling of the trough between 2 lines of a doublet of coupled lines of symmetry F1 ↔ F2**

P9

Mean spectral from retrieved state (Robs, Rcalc)



Mean spectral residuals from retrieved state (obs – calc)



Hawaii retrievals on L1(IASI)

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  1246 cm^{-1} → P9 multiplet (previous slide); and 1268 cm^{-1} → P6 multiplet (this slide)
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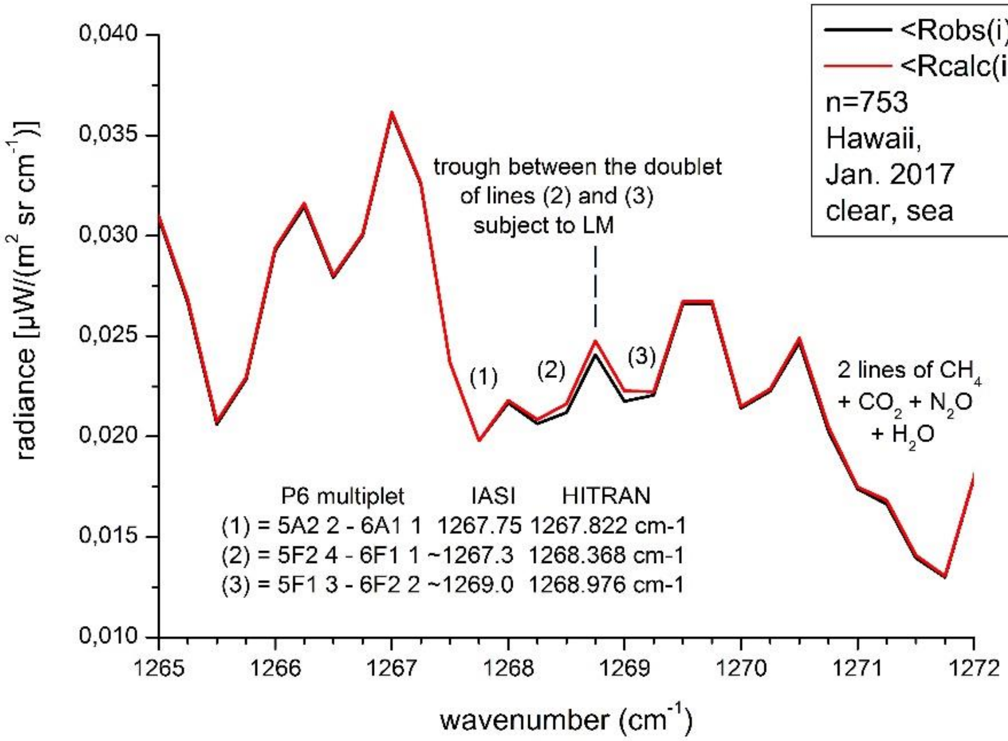
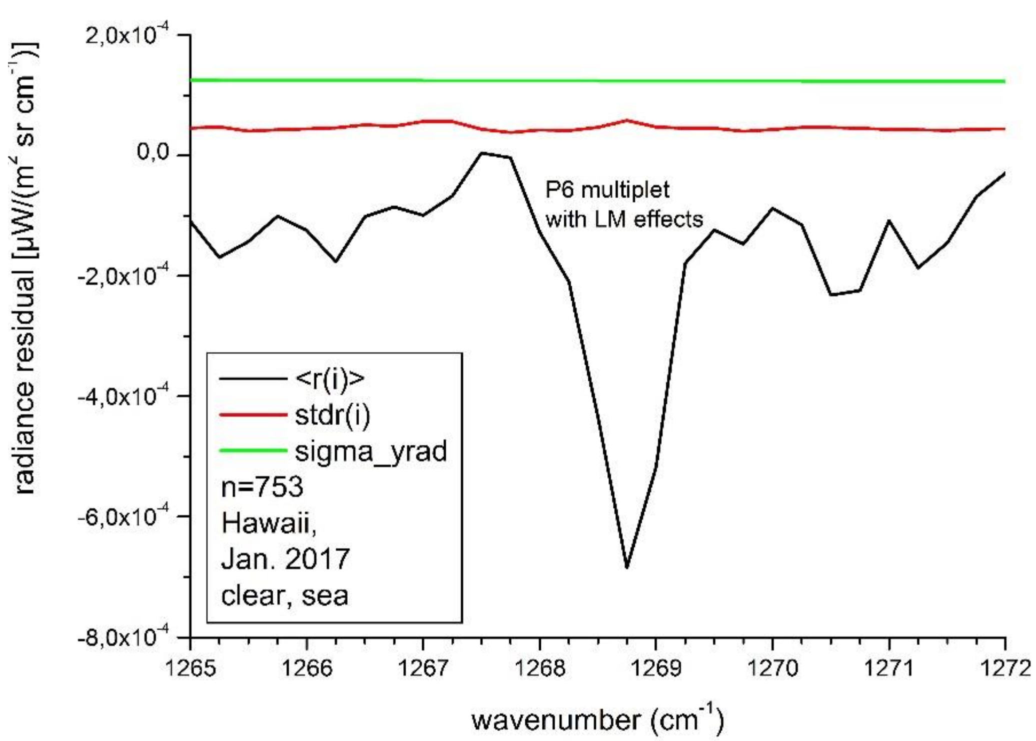
P6

Mean spectral from retrieved state (Robs, Rcalc)



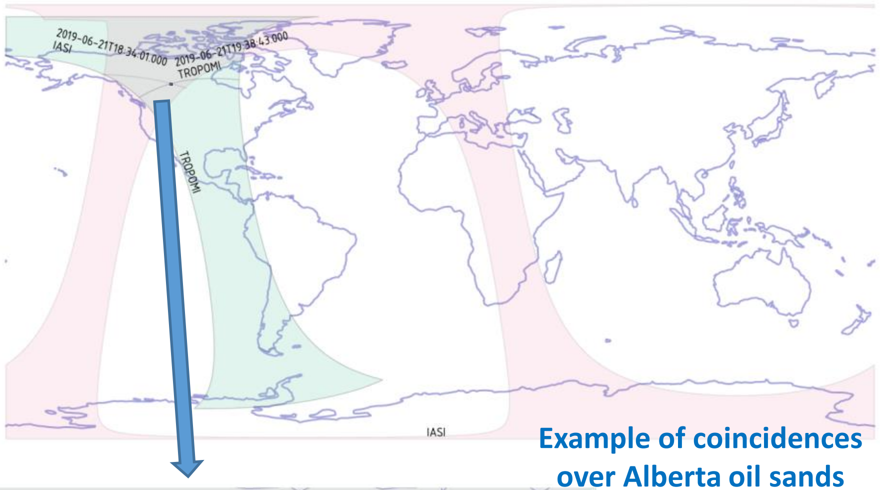
Mean spectral residuals from retrieved state (obs – calc)

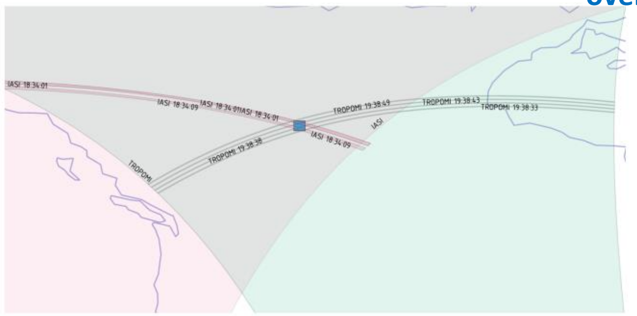


Algorithm implementation for application to real data

- **Work is ongoing for L1(IASI) and L2(TROPOMI) comparison, then synergistic retrievals …**

Spatio-temporal coincidences between IASI and TROPOMI exist. More favourable in high latitudes.





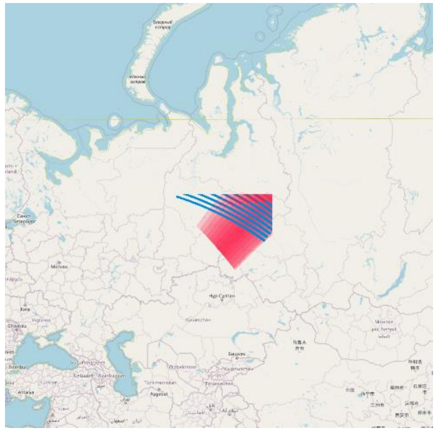
Example of coincidences over Alberta oil sands region

90 coincidences found in this region () between June and September 2019, with a time tolerance of 1 hours. The 10 best are listed below

Δt (h)	TROPOMI	IASI
0,11	2019-08-16 18:42:05	M02 2019-08-16 18:49:14
0,15	2019-07-14 18:58:03	M02 2019-07-14 19:07:35
0,19	2019-07-15 18:37:23	M02 2019-07-15 18:49:03
0,22	2019-07-16 18:16:43	M02 2019-07-16 18:30:30
0,24	2019-06-08 18:28:25	M02 2019-06-08 18:43:07
0,28	2019-06-09 18:07:45	M02 2019-06-09 18:24:37
0,28	2019-09-07 18:20:04	M02 2019-09-07 18:37:01
0,32	2019-07-19 18:54:34	M02 2019-07-19 19:13:50
0,35	2019-07-20 18:34:02	M02 2019-07-20 18:55:13
0,37	2019-09-10 18:57:55	M02 2019-09-10 19:20:20

A dataset of coincident TROPOMI and IASI data, together with ECMWF/CAMS fields, has been collected over Siberia for summer 2019

L1(IASI) CH_4 retrieval is ongoing …



Example of Observations for the 5th June 2019 IASI 05:59 (blue) vs TROPOMI 06:08 (red)

Next steps :

- Comparisons with L2(TROPOMI and statistical analysis of the differences
- L1(IASI)+L2(TROPOMI) retrievals
- Application on different region for testing consistency
- Retrieval over test cases with correlative data

Thank you for your attention !

Questions and comment are welcome

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Algorithm implementation for application to real data

- **OEM formalism for L1(IASI) + L2(TROPOMI), with 4A/OP forward model: cost function**

$$\chi^2 = (\mathbf{y} - \mathbf{f}(\mathbf{x},\mathbf{b}))^T \mathbf{S}_y^{-1}(\mathbf{y}-\mathbf{f}(\mathbf{x},\mathbf{b})) + (Y - F(\mathbf{x},\mathbf{b},\mathbf{b'},\mathbf{x}_a'))\, S_Y^{-1}\, (Y - F(\mathbf{x},\mathbf{b},\mathbf{b'},\mathbf{x}_a')) + (\mathbf{x}-\mathbf{x}_a)^T\mathbf{S}_x^{-1}(\mathbf{x}-\mathbf{x}_a)$$

y = observation **vector** for TIR (extract of the L1C IASI spectrum)
$\mathbf{S}_y$ = uncertainty covariance matrix for TIR (possibly accounting for forward model errors)
f = observation operator for TIR (forward model for **vector y**)

b = **vector** of auxiliary variables for TIR (thermodynamics i.e. T(i), P(i) on the TIR retrieval grid and other non retrieved parameters)

x = state **vector** (vertical mixing ratio profile of CH_4)
$\mathbf{x}_a$= *a priori* state **vector**
$\mathbf{S}_a$ = covariance matrix of the *a priori* uncertainty of the state vector

Y = SWIR observation scalar (column averaged dry air CH_4 mixing ratio, SWIR L2 product)
F = observation operator for SWIR (direct model for computing the scalar Y)
S_Y = observation uncertainty for SWIR (a scalar)
b' = **vector** of auxiliary variables for SWIR (thermodynamics i.e. T(i), P(i) on the SWIR retrieval grid and other non retrieved parameters)
$\mathbf{x}_a'$= *a priori* state **vector** used for generating the L2 product (one may need it for the forward model computation of Y)