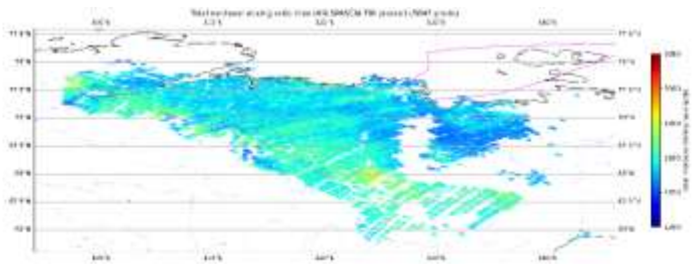
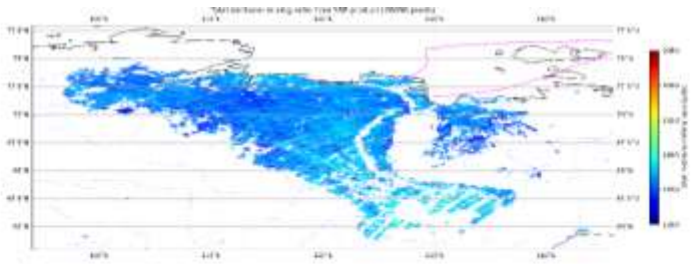
Potential of TIR+SWIR combination from space measurements for CH_4 retrievals: synergy between IASI and S5P

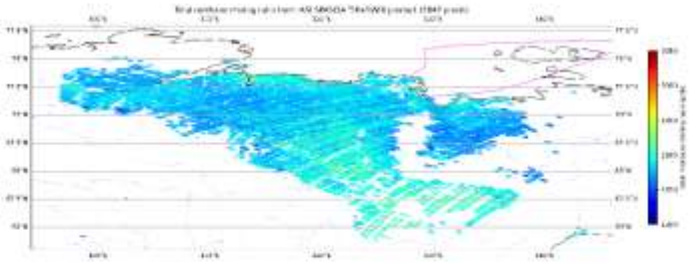
XCH_4 IASI TIR



XCH_4 S5P



XCH_4 IASI TIR+SWIR



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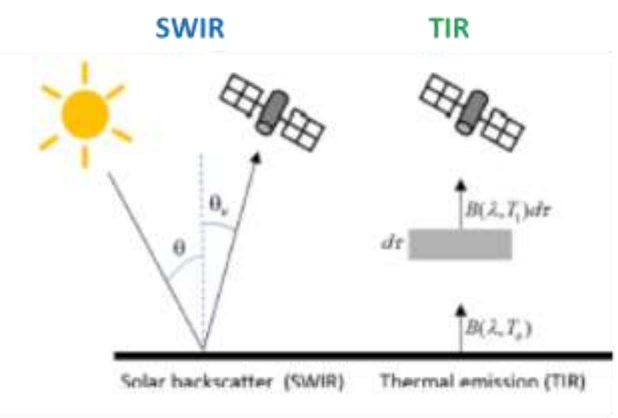
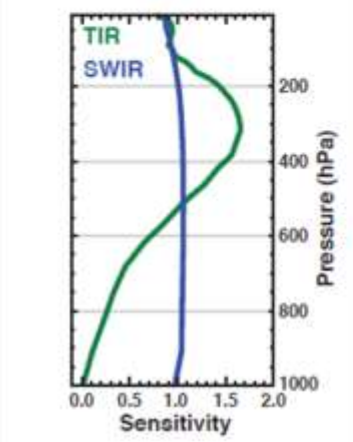
IASI conference, December 2024, Nancy

Introduction

Atmospheric CH_4 is measured continuously from space-borne passive optical instruments.

- Instruments in the SWIR provide a total atmospheric column with rather uniform sensitivity up to the tropopause (including the lowermost layers).
  - Past and current : SCIAMACHY, 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 : 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

Spectral synergies for CH_4

Expected added-values of the synergy between IASI and TROPOMI (preparing IASI-NG/S5 UVNS)

- Analyse differences and improve consistency between TIR and SWIR products
- Improve vertical information with better sensitivity to the surface by combining the two products
- Provide a unique and consistent product over land/ocean and night/day

Already existing work/products combining L2 products : KIT (Schneider et al., 2021) and RAL (ESA PROMCOM project)

TIR L1(IASI) + SWIRL2(TROPOMI) Algorithm implementation

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

$$\chi^2 = (\mathbf{y} - \mathbf{f}(\mathbf{x},\mathbf{b}))^T \mathbf{S_y}^{-1}(\mathbf{y}-\mathbf{f}(\mathbf{x},\mathbf{b})) + (X_{CH_4}^{S5P} - F(\mathbf{x},\mathbf{b},\mathbf{b'},\mathbf{x_a'}))\, S_Y^{-1}\, (Y - F(\mathbf{x},\mathbf{b},\mathbf{b'},\mathbf{x_a'})) + (\mathbf{x}-\mathbf{x_a})^T\mathbf{S_x}^{-1}(\mathbf{x}-\mathbf{x_a})$$

- **S5P/TROPOMI introduction in the TIR+SWIR inversion**

TROPOMI pixels inside a IASI pixel are averaged to a column averaged mixing ratio $X_{CH_4}^{S5P}$ and added as one L2 observation in the inversion

An observation operator F is used to compute $X_{CH_4}^{S5P}$ from CH_4 profile x:

$$X_{CH_4}^{S5P} = F(x, b, b', x_a) = C.\frac{\sum_i x_i w_i^{S5P} \Delta p_i}{\sum_i w_i^{S5P} \Delta p_i}$$

Here C is a scaling factor introduced to take into account a possible inconsistency between TIR and SWIR measurements. It has been parametrized with a value of 0.992 by an *ad hoc* procedure.

The w_i^{S5P} are the weights provided in the S5P CH_4 L2 product.

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)

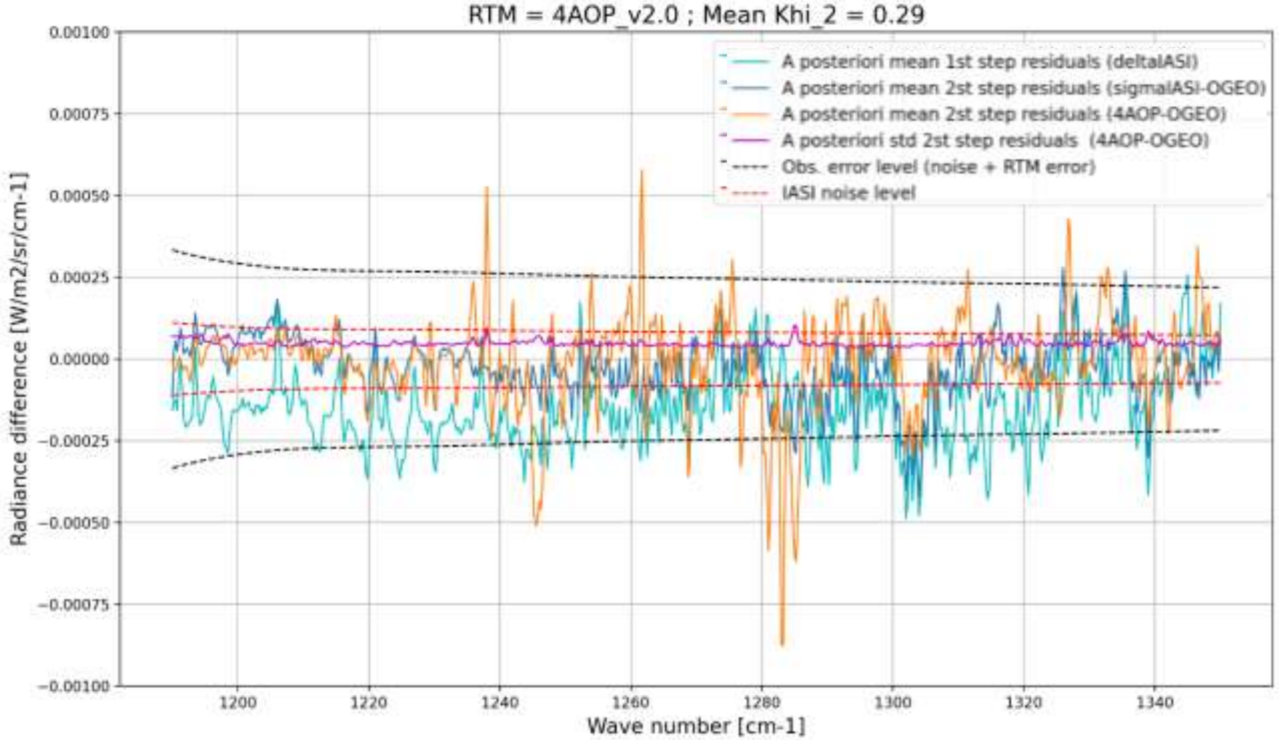
x = state **vector** (vertical mixing ratio profile of CH_4)
$\mathbf{x_a}$= *a priori* state **vector**
$\mathbf{S_a}$ = covariance matrix of the *a priori* uncertainty of the state vector

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)

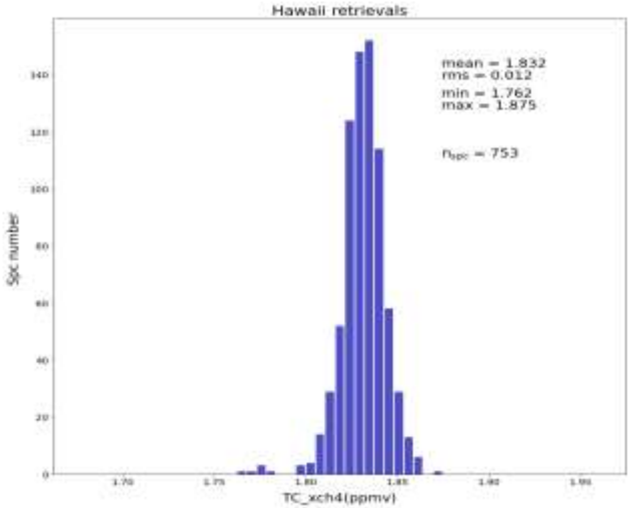
OEM CH_4 TIR retrieval algorithm validated with IASI

- Based on OGEO OEM retrieval scheme and 4AOP radiative transfer model
- Retrievals from IASI L1C spectra over **Hawaii, January 2016** : validation and intercomparison of UniBas, BIRA and SPASCIA algorithms including a comprehensive analysis and improvement of spectroscopy biases and uncertainty (ESA CH4TIR projet, 2021)*)*

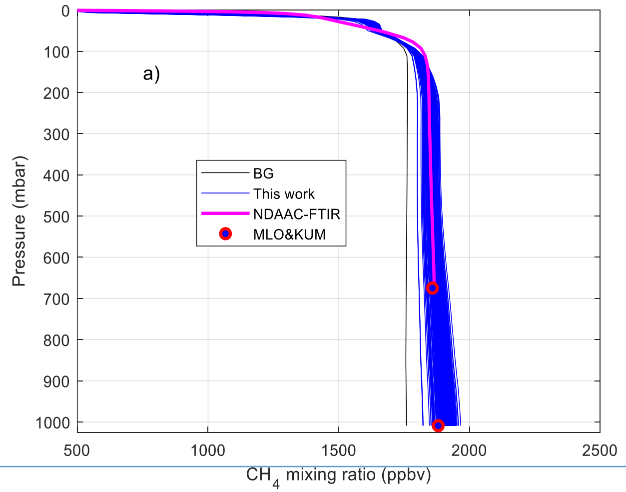
Mean spectral residuals from retrieved state (obs – calc) for different versions of algorithms



Small spectral residuals with some identified peaks (CF_4 molecule not in 4A/OP at 1283 cm^{-1} and line-mixing effects for other peaks)



XCH_4 retrievals

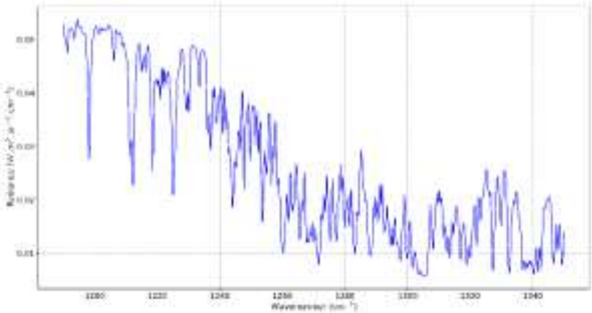


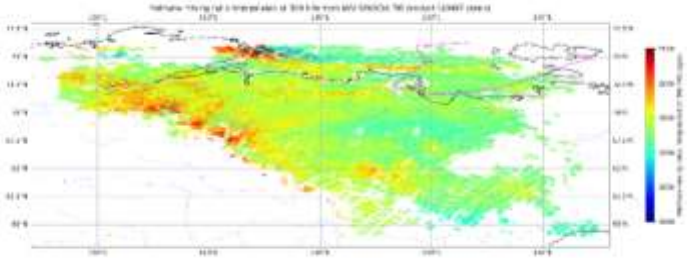
CH_4 profile retrievals compared with reference data (NDACC and *in situ*)

Retrieval over Siberia : satellite and in situ airborne data

- Analysis over a large region in Siberia (55N-78N, 40E-190E)
- Comparing with available correlative measurements from YAK-AEROSIB September 2020 campaign (data provided by J.-D. Paris and C. Narbaud).

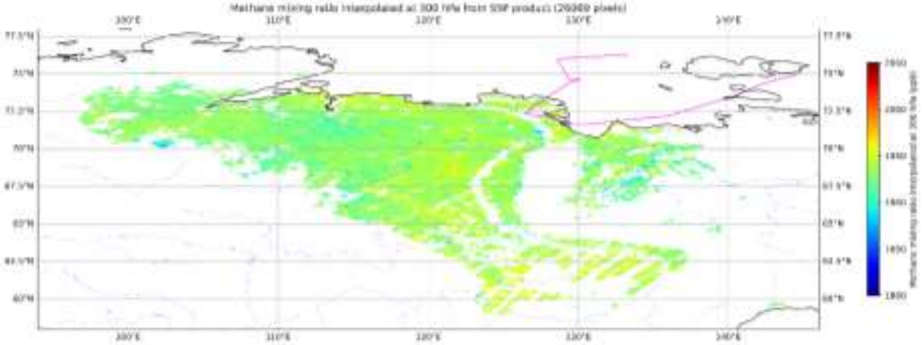
IASI L1C spectra
Radiance spectra of IASI L1C between 1190 and 1350 cm^{-1}





Example of IASI LC spectra for one pixel close to airborne campaign, and Methane mixing ratio interpolated at 300 hPa

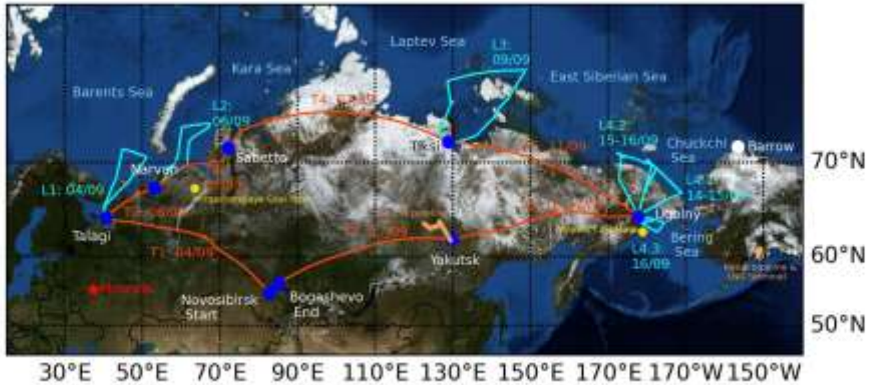
Sentinel-5P product
Reprocessed product created in Nov. 2022 (algorithm version 1.5.0)



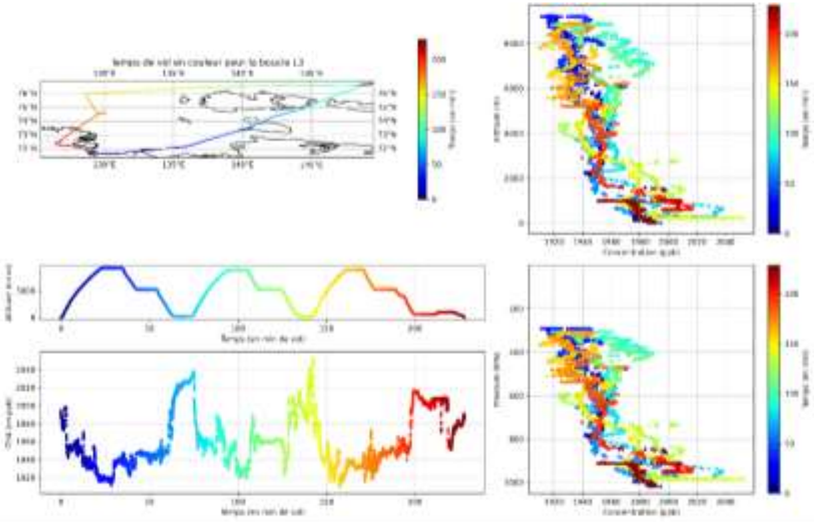
L2 S5P/TROPOMI Methane mixing ratio (interpolated at 300 hPa from CH_4 vertical profile)

Available correlative *in situ* profile observations

YAK-AEROSIB campaign, 4-17 September 2020, 13 flights over different areas of the region. Narbaud et al., 2022



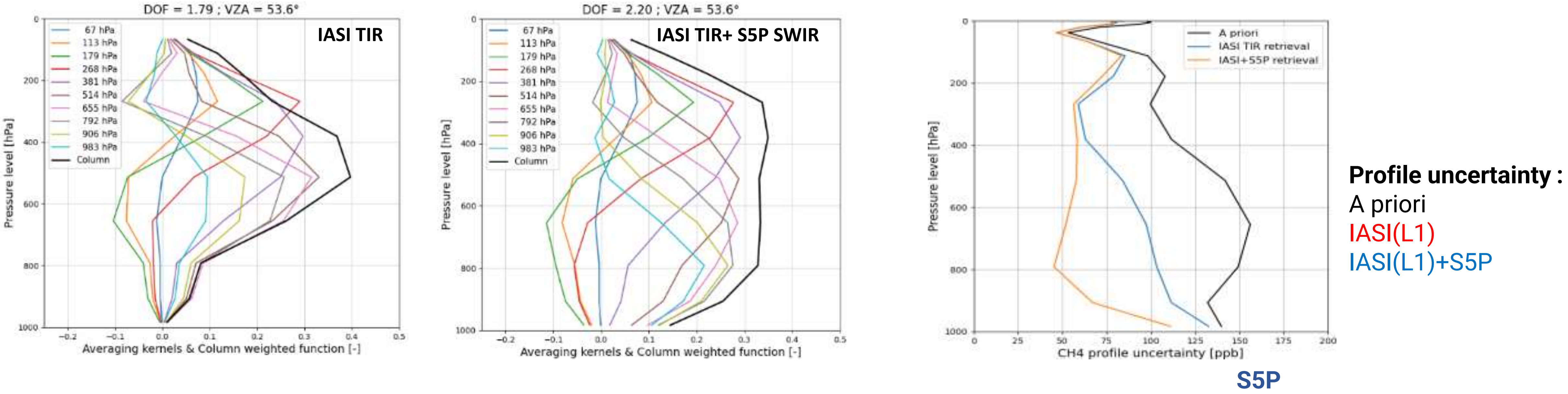
From Narbaud et al., 2022 September 2020 campaign flight plan. The 13 flights are indicated either as "loop" (prefix L, cyan line) or "transit" (prefix T, orange line).



YAK-AEROSIB campaign data for loop L3. ground track of the aircraft's path, time evolution of altitude and CH4 mixing ratio, vertical profiles of CH4 mixing (colour is the flith time)

Information content analysis with EOM

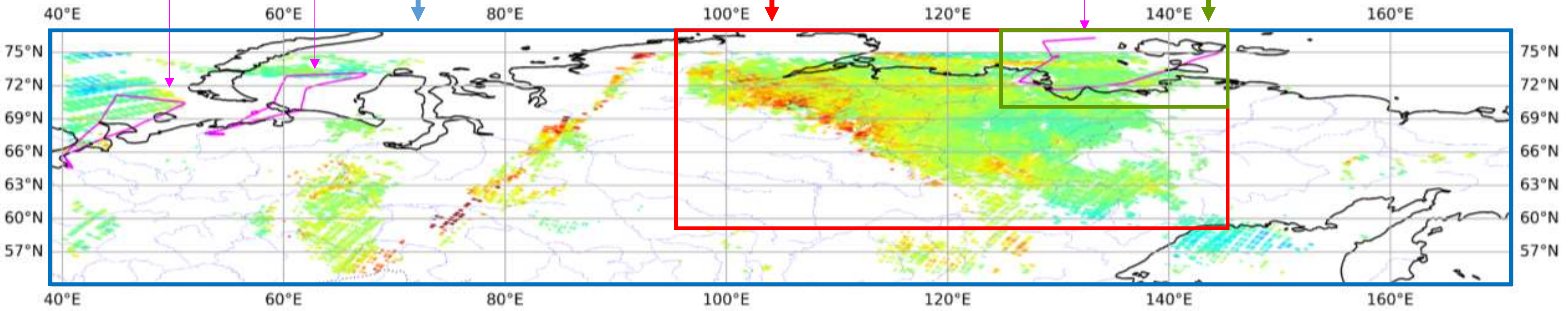
- Exemple of averaging kernels in Siberian region : CH_4 profile information (between 200 and 600 hPa) can be retrieved from IASI observations with a Degree of Freedom of 1.8. From IASI L1C spectra + L2 S5P retrieval synergy, the CH_4 profile sounding is extended down to lower layers (around 800 hPa) with an associated DOF around 2.2 in this case.

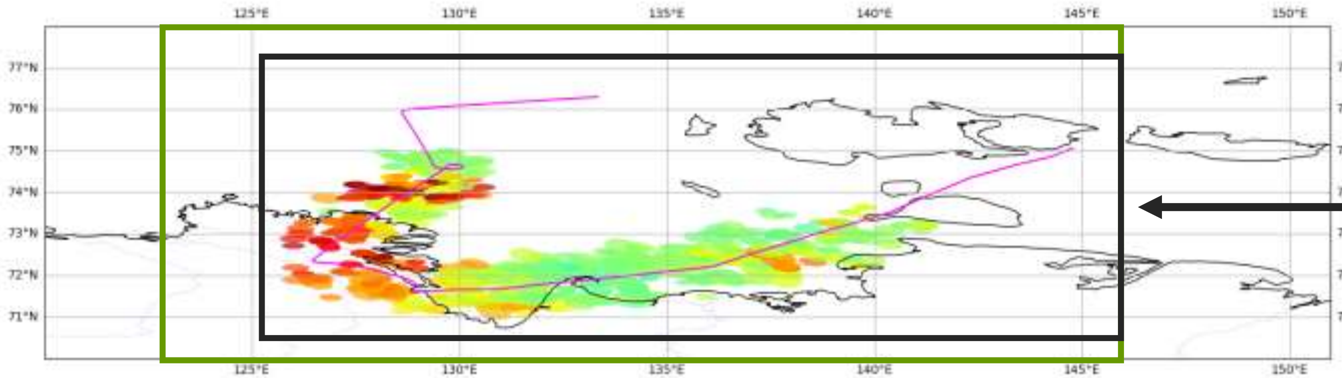


- significant gain of uncertainty reduction in the lower troposphere between IASI TIR retrieval and IASI TIR+SWIR retrieval.

- Boucles sur la zone et différentes zones d'étude

L1 L2 Zone complète Zone zoomée L3 L3 Zone proche L3

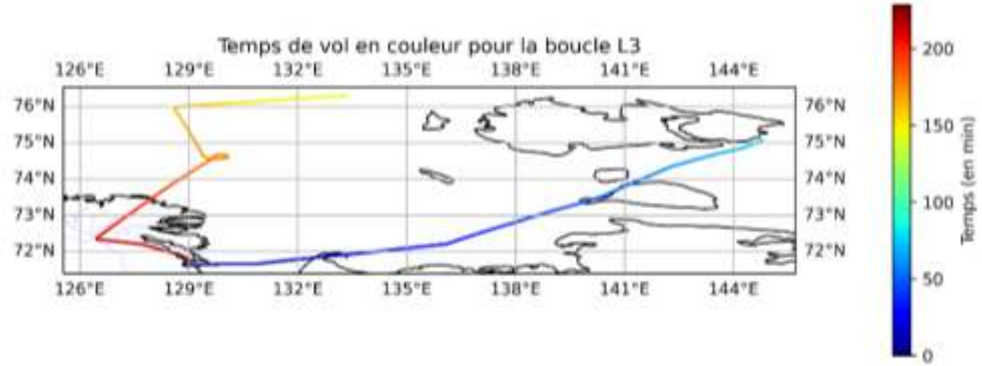


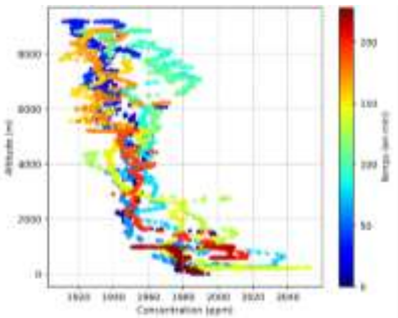


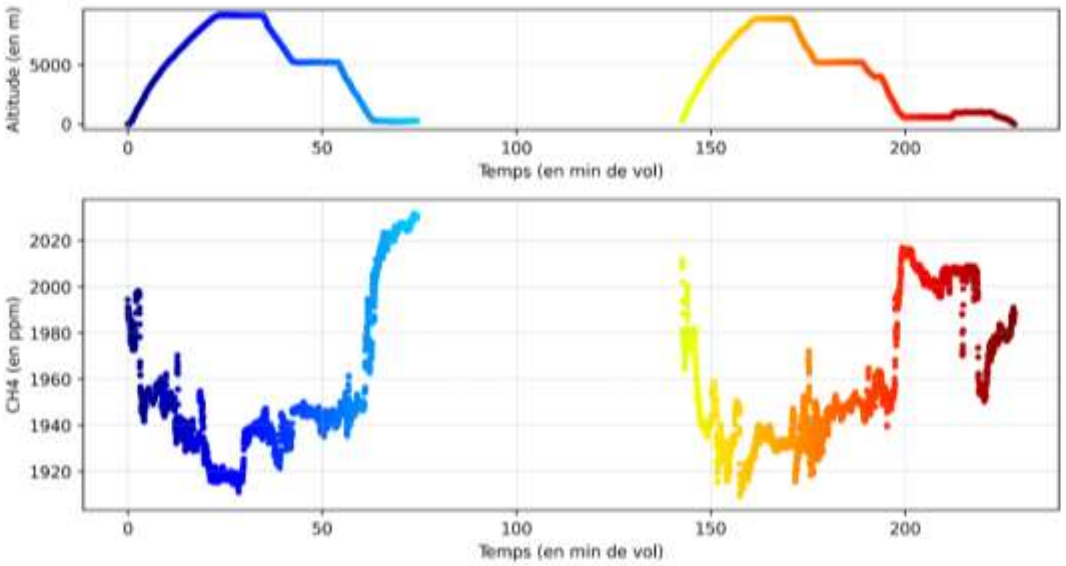
Zone coïncidence L3

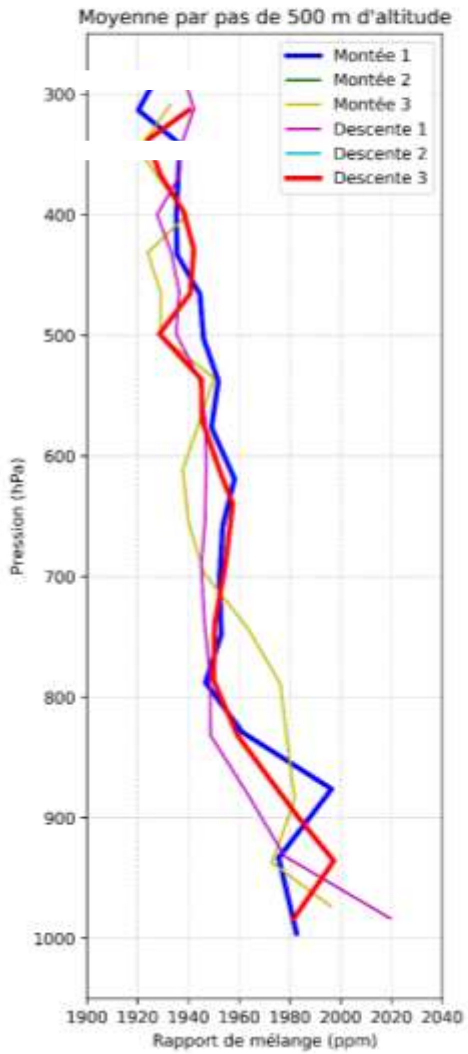
Focus on loop L3 of the YAK-AEROSIB campaign : correlative dataset used

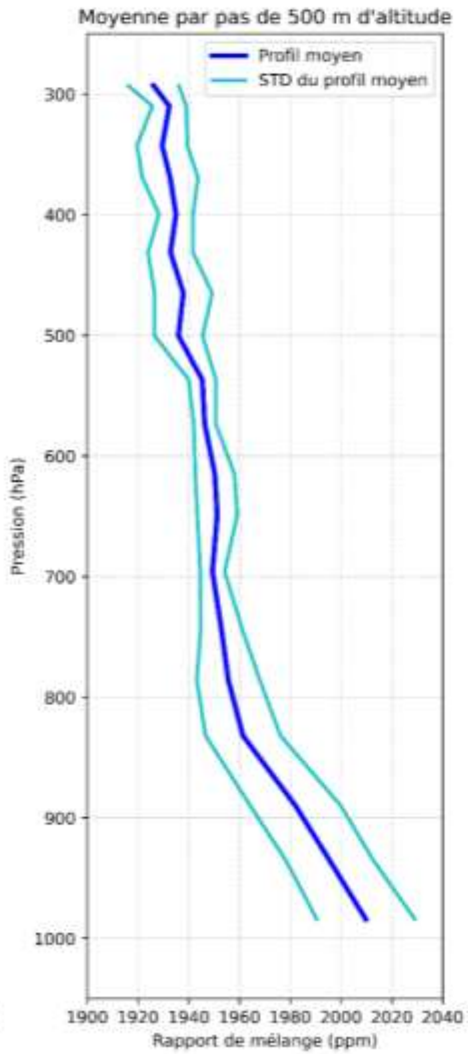
➢ We selected the correlative measurements where satellite data area available

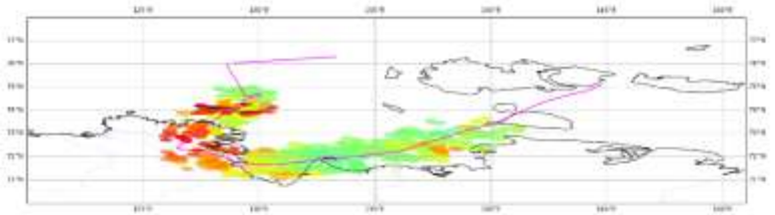








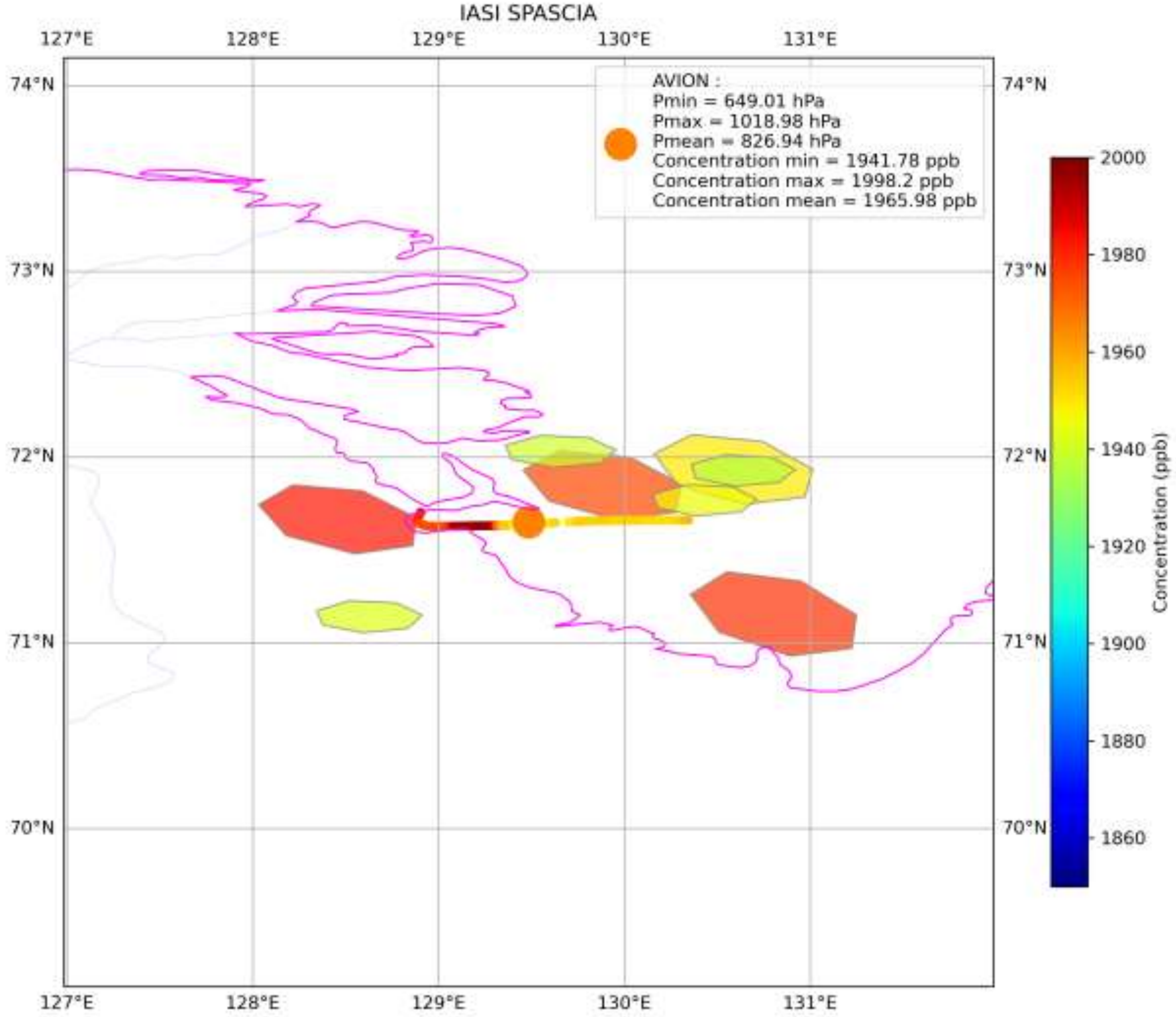


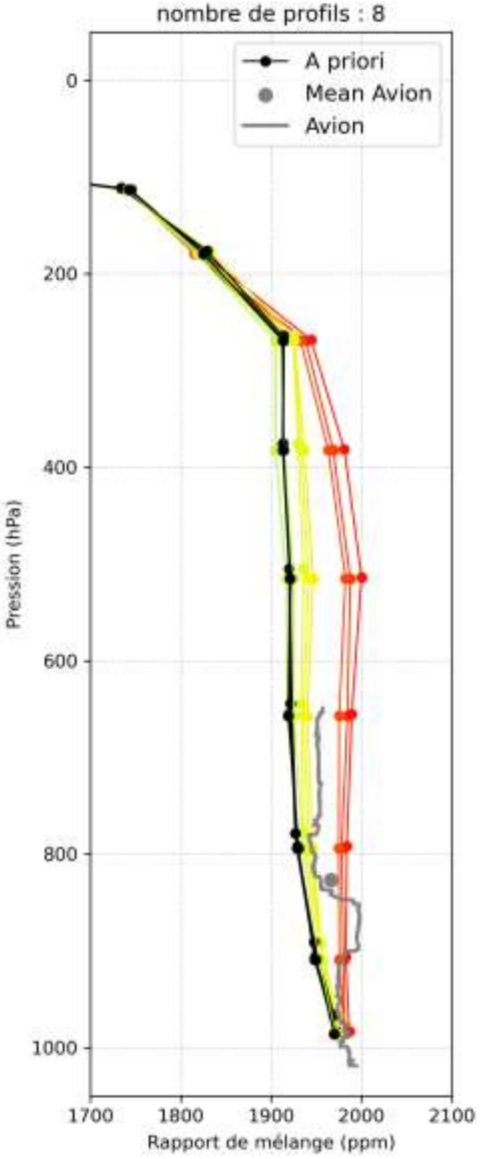


Focus on loop L3 of the YAK-AEROSIB campaign : IASI TIR profile retrieval

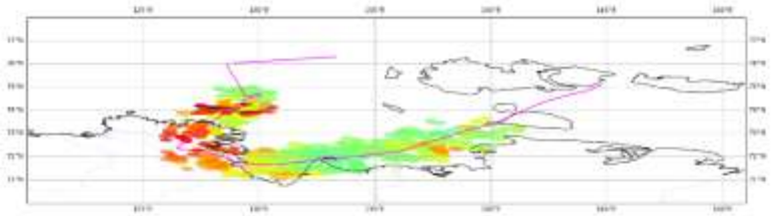
Retrieval at the aircraft's flight path (Loop L3) :

- **on the left-hand side, we show the interpolated mixing ratio map at the aircraft's mean pressure over the flight section for the inverted IASI pixels and the concentration measured by the aircraft.**
- **On the right-hand side, we show the vertical profiles of the *a priori* in black and the retrievals in colour (associated with the pixel colour on the left) and the vertical profile of the aircraft concentration (in grey).**
- **All quantities are in ppb.**



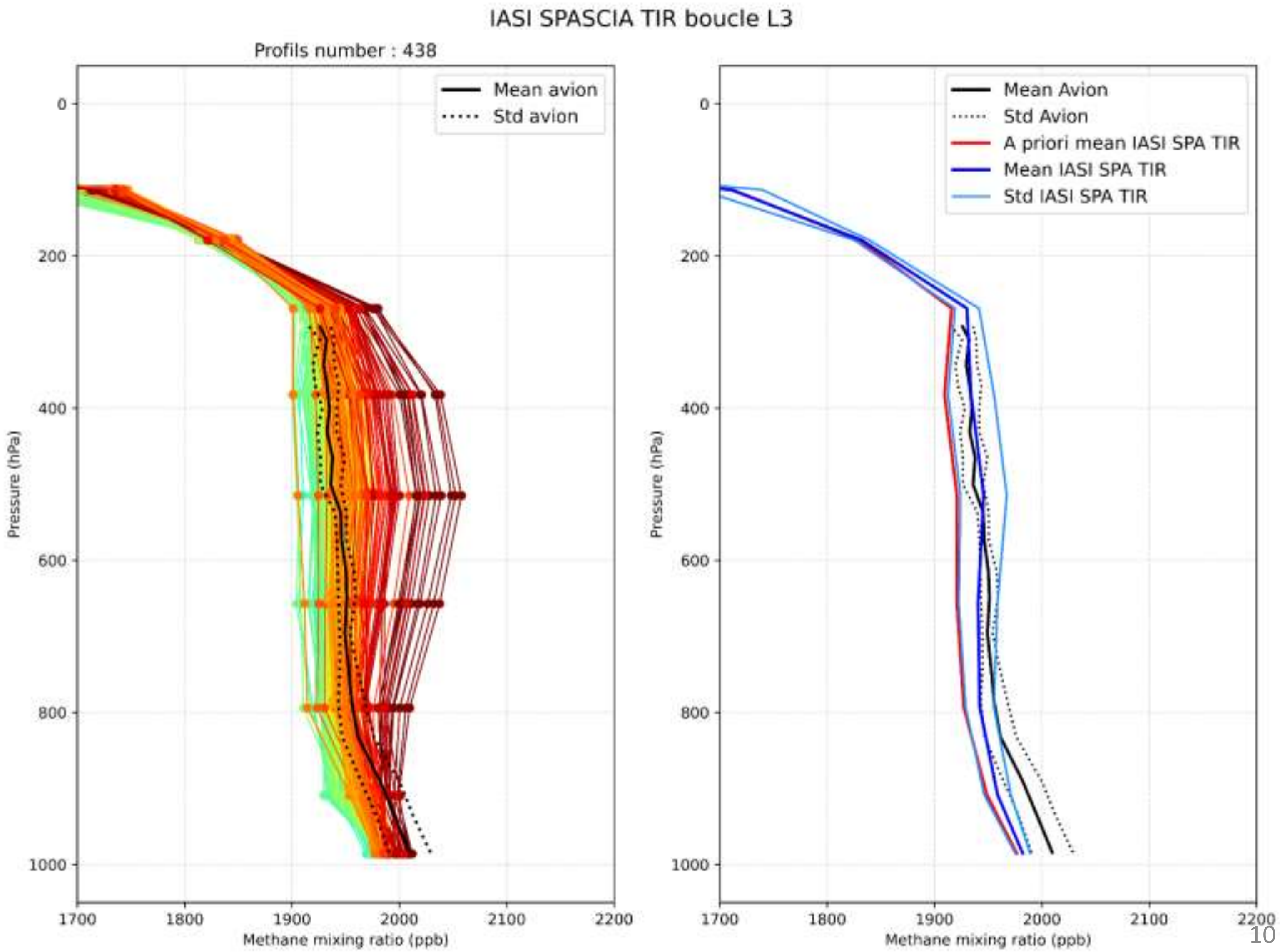


SPASCIA

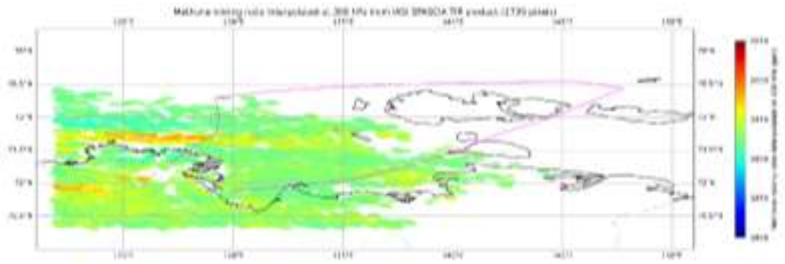


Focus on loop L3 of the YAK-AEROSIB campaign : IASI TIR profile retrieval

- 438 retrieved profile from IASI close to the L3 loop
- Good agreement with corelative profile measurements.
- In the presented results, retrievals outliers are not post-filtered. To be done based on χ^2. provided by OEM.



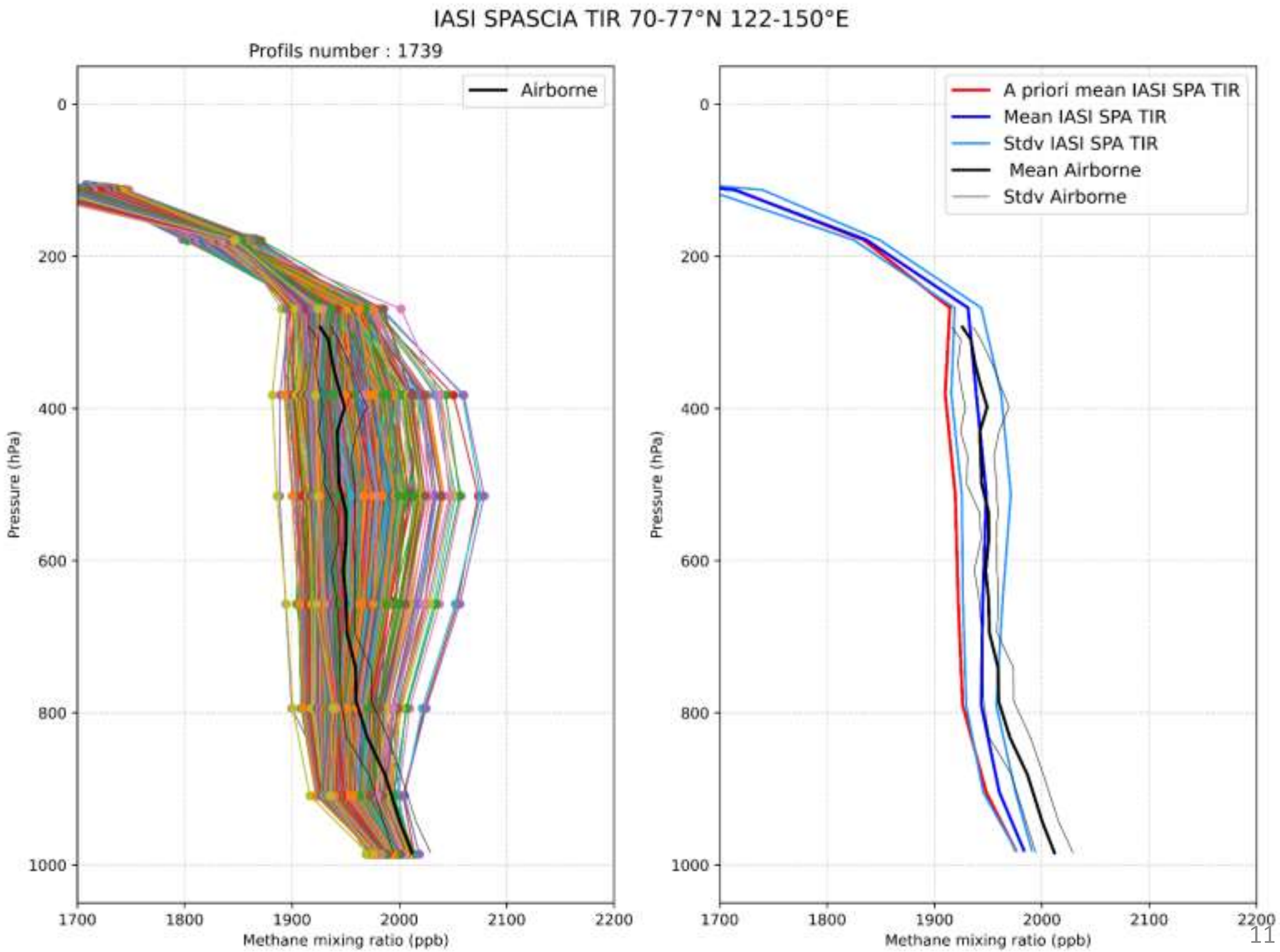
SPASCIA



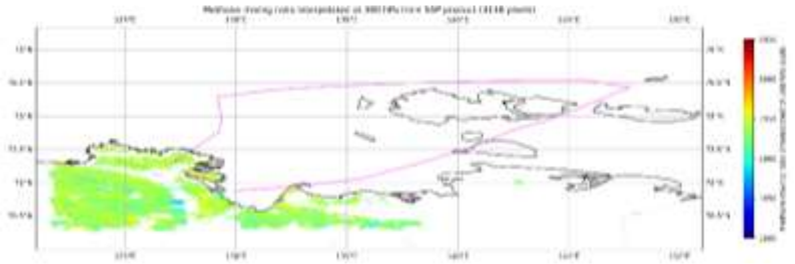
Larger zone close to loop L3 of the YAK-AEROSIB campaign : IASI TIR profile retrieval

A larger zone is considered for next step : synergy retrievals with S5P/TROPOMI :

- ➢ 1739 retrieved profile from IASI considered in a larger zone, good agreement remains with corelative profile measurements.



SPASCIA

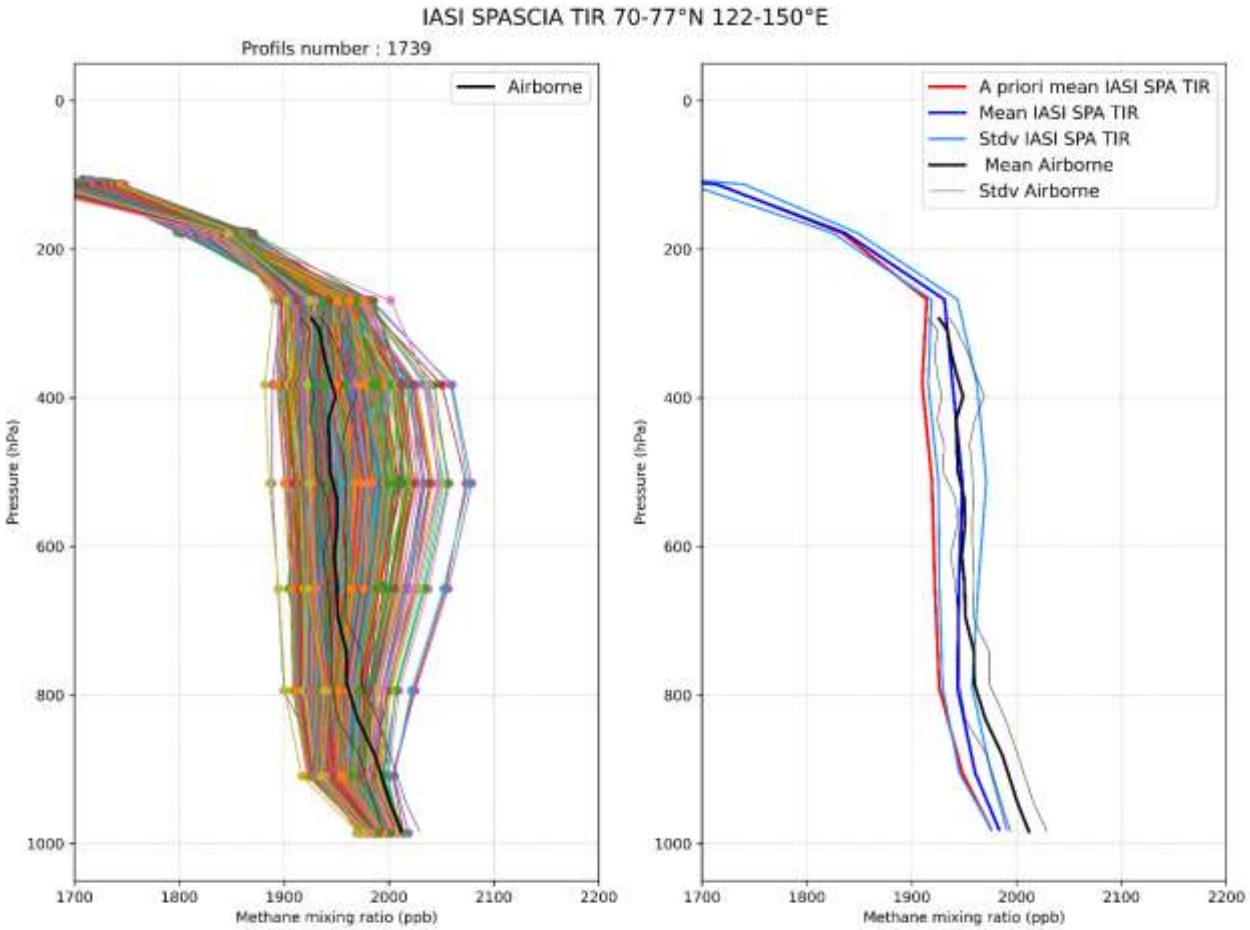


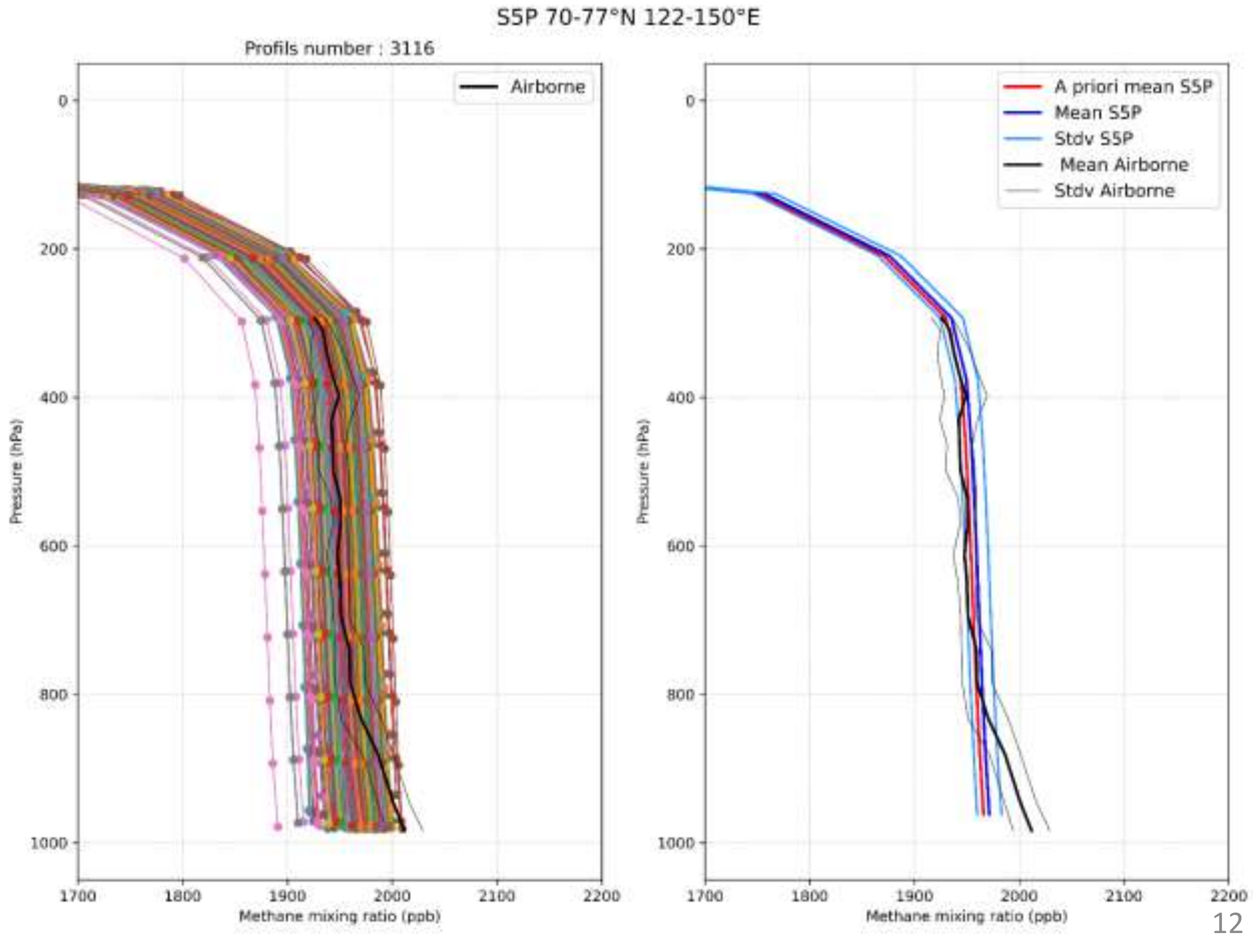
Larger zone close to loop L3 of the YAK-AEROSIB campaign : Coïncident IASI TIR profile retrieval and S5P products

IASI TIR profile retrievals

S5P product (column mixing ratio)

Profiles reconstructed from a priori and column mixing ratio product



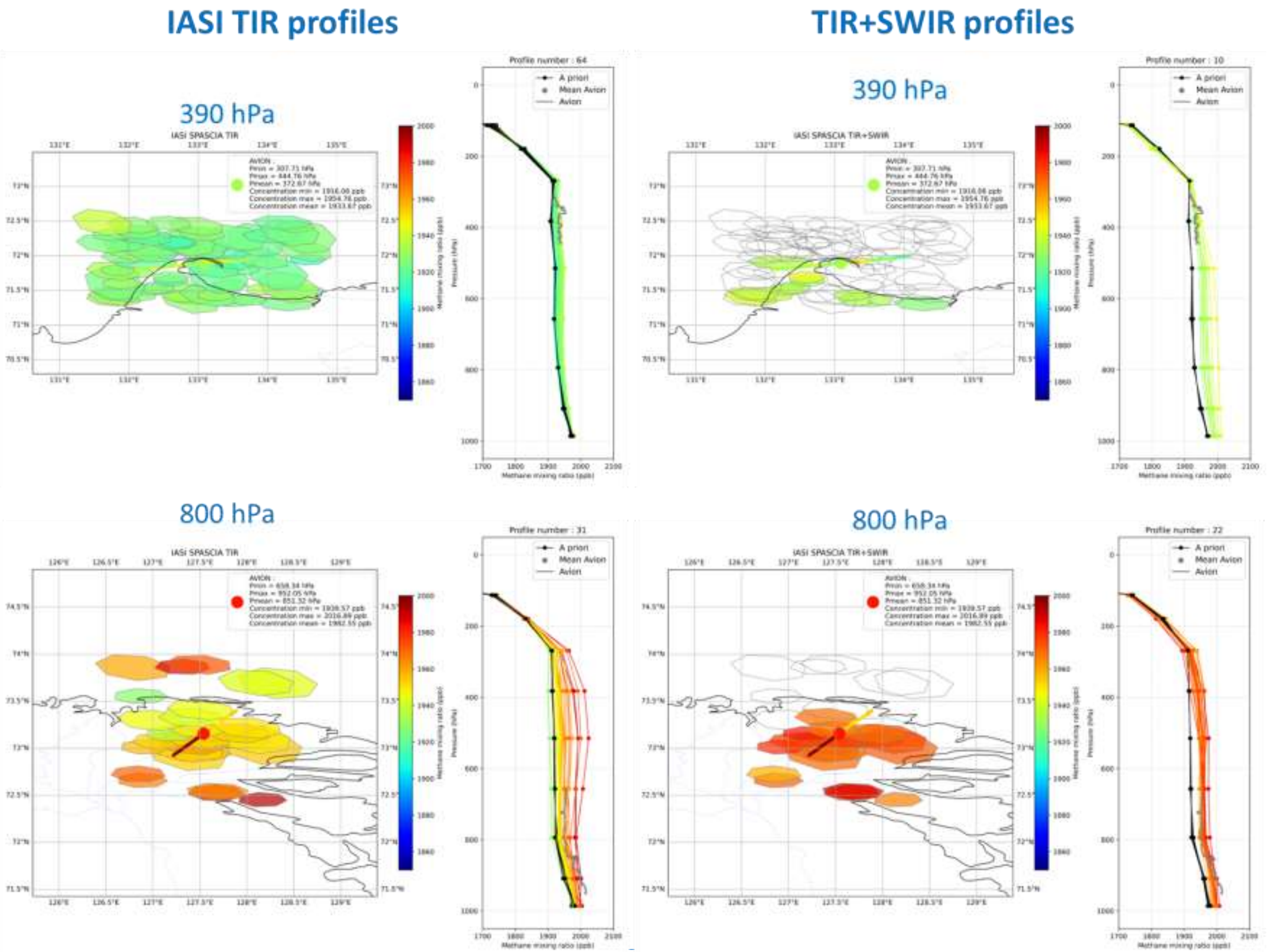


TIR+SWIR retrievals from IASI and S5P

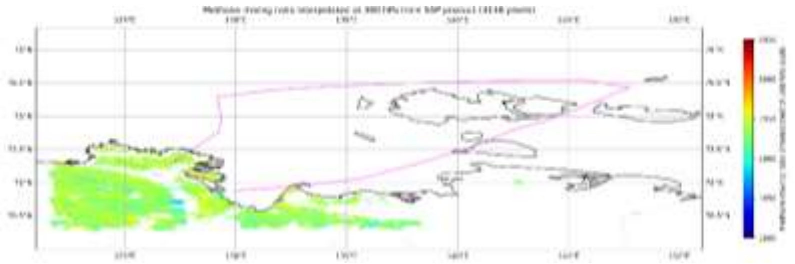
The vertical profiles of IASI inversions are, in principle, already in good agreement with the in situ measurements of the airborne campaign, in both the lower and upper parts of the atmosphere.

The vertical profiles obtained from the synergistic inversion of IASI and S5P are improved:

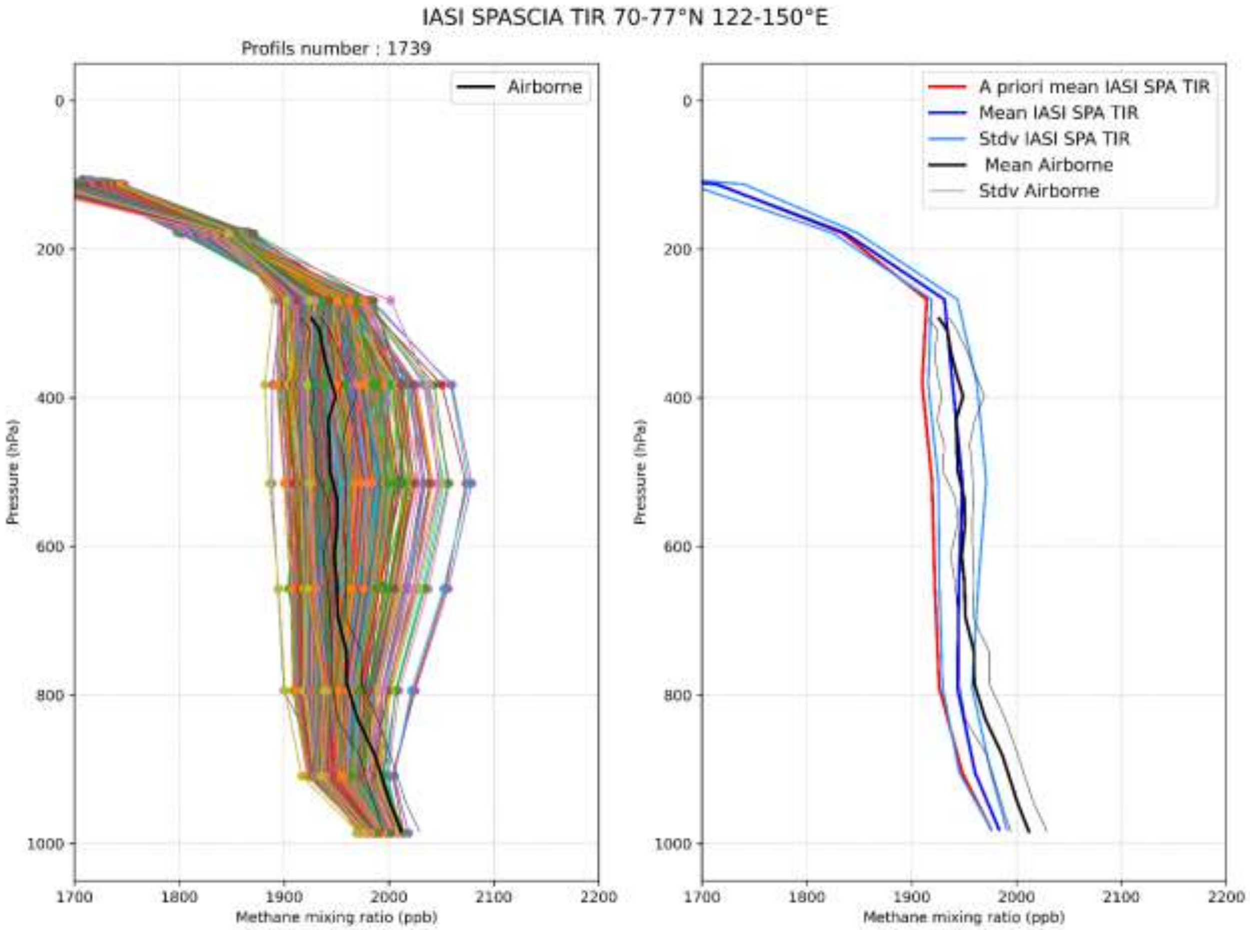
- closer to the reference profiles,
- more constrained by the measurements (further from the a priori),
- less dispersed.



Larger zone close to loop L3 of the YAK-AEROSIB campaign : Coïncident IASI TIR profile retrieval and S5P products

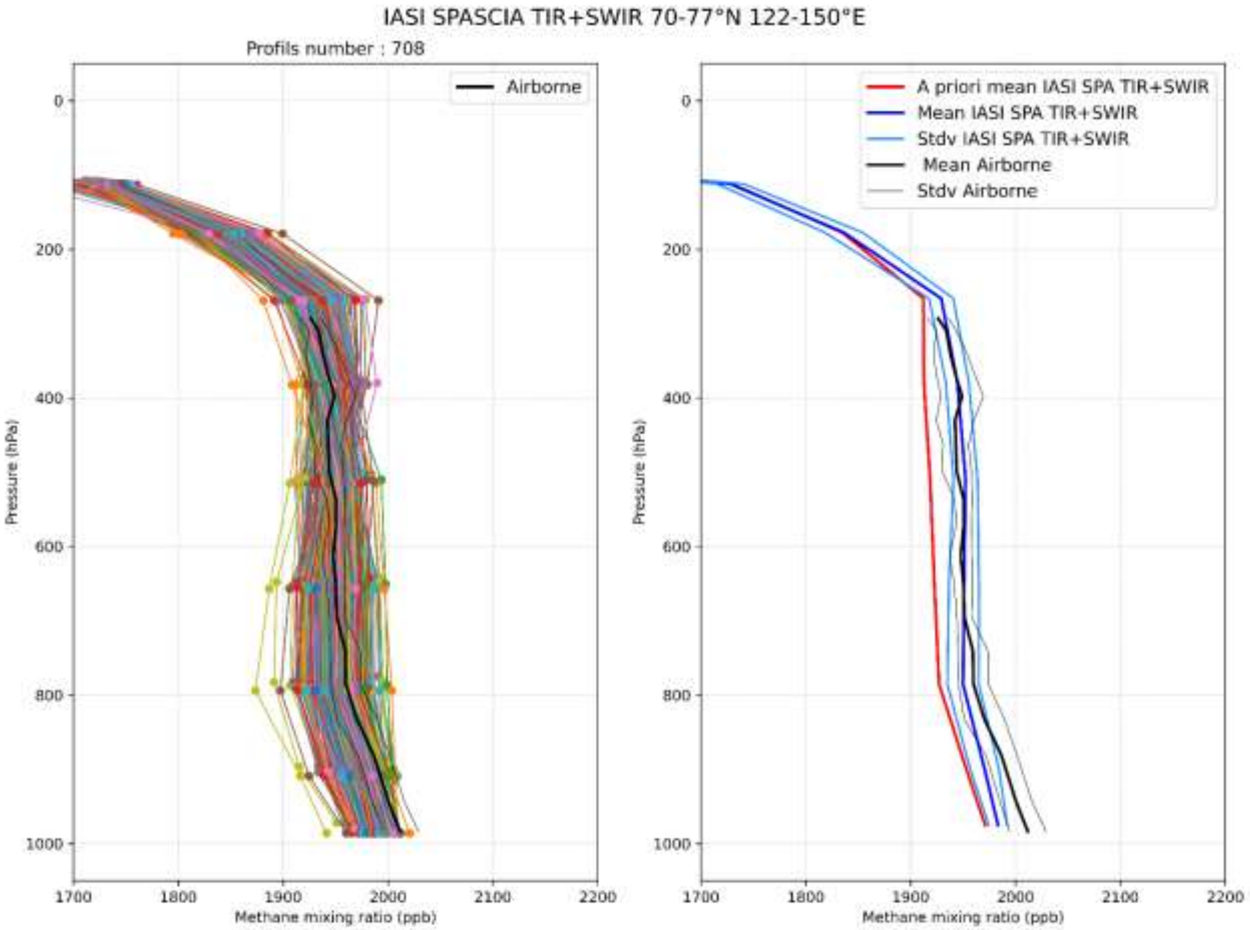


IASI TIR profile retrievals



IASI TIR + S5P SWIR retrievals

708 pixels

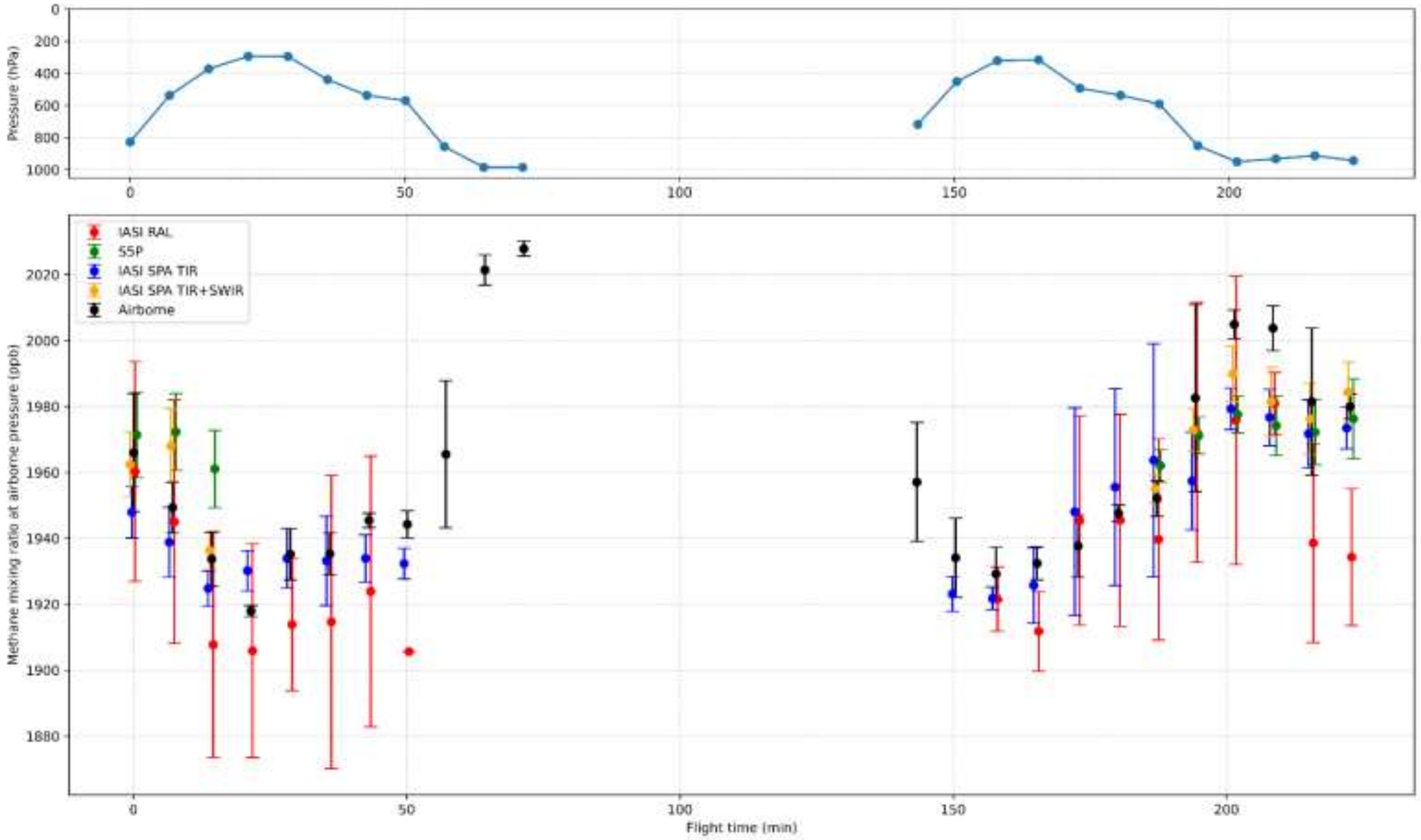


Comparison of the CH4 mixing ratio at the pressure of the airborne measurement

Airborne data, IASI TIR (SPASCIA), IASI TIR (RAL), S5P, IASI TIR+SWIR

Comparison of the CH_4 mixing ratio at the pressure of the airborne measurement over Loop L3 as a function of the flight time :

- ➢ The spatio-temporal and vertical variations of the *in situ* measurements are well reproduced by both TIR and TIR+SWIR retrievals.
- ➢ In addition, the TIR+SWIR retrievals exhibit improved agreement with airborne data in the lowermost part of the atmosphere (as shown in the last part of the time series from 200 mn flight time onwards)

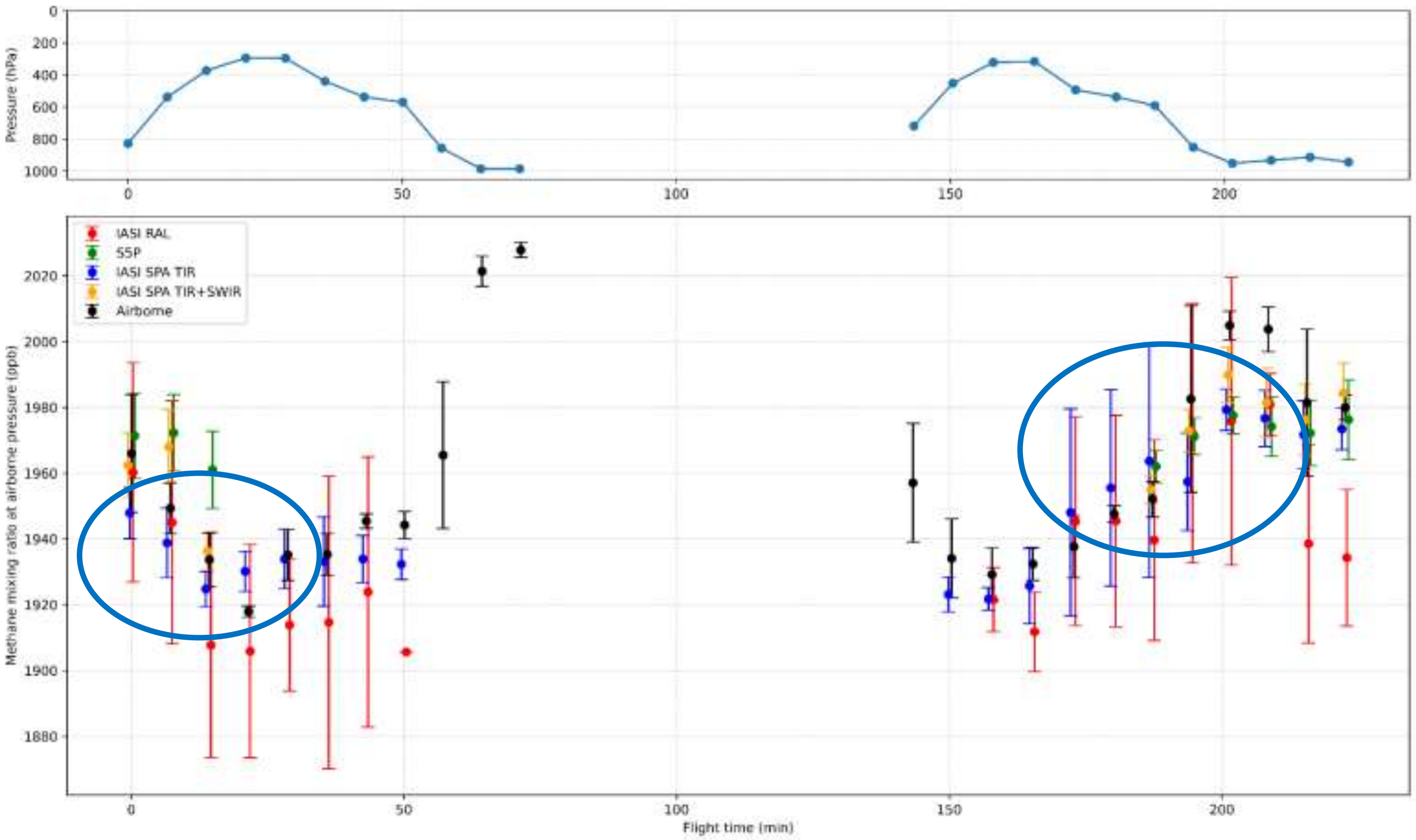


Comparison of the CH4 mixing ratio at the pressure of the airborne measurement

Airborne data, IASI TIR (SPASCIA), IASI TIR (RAL), S5P, IASI TIR+SWIR

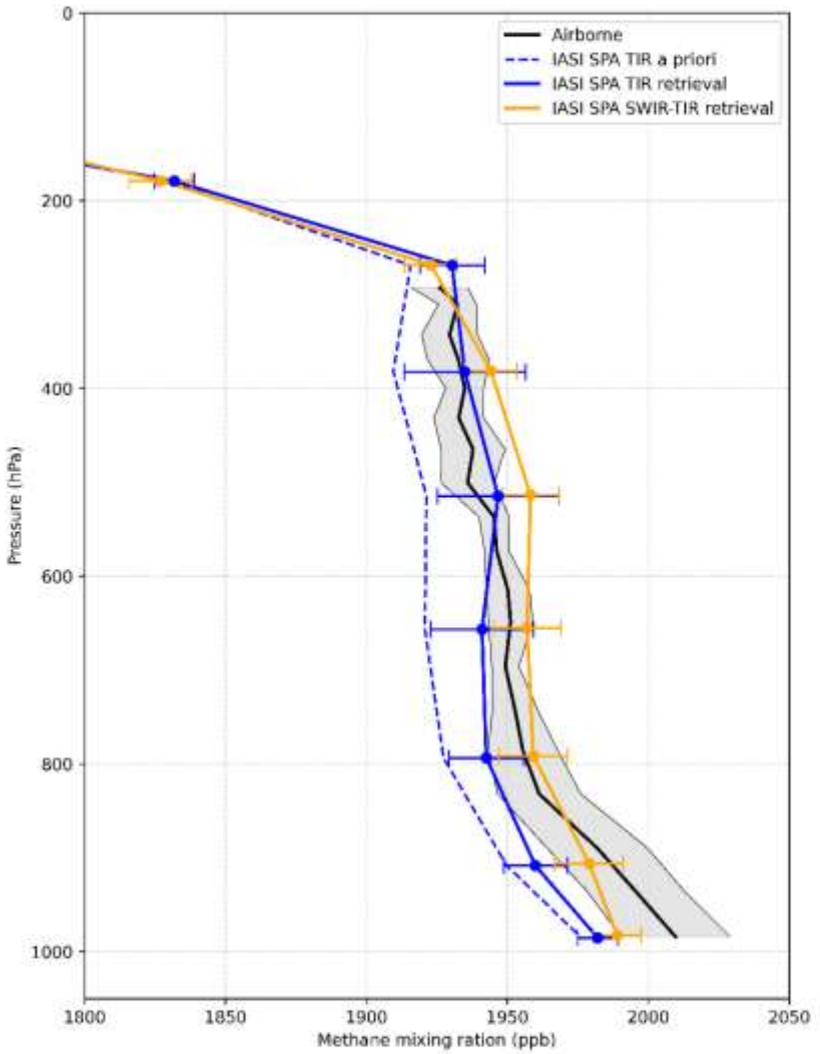
Comparison of the CH_4 mixing ratio at the pressure of the airborne measurement over Loop L3 as a function of the flight time :

- A remarkable continuity of the IASI+S5P and IASI-only time series is observed at land-sea transitions, when synergistic restitution is no longer possible due to a lack of S5P data, and TIR inversion takes over.
- This suggests that it will make it possible to provide coherent atmospheric CH4 concentration data that can be used continuously under different conditions, whether they are favorable to TIR or SWIR (land-sea transitions, night-day).



Discussion

- Mean profiles on the L3 loop

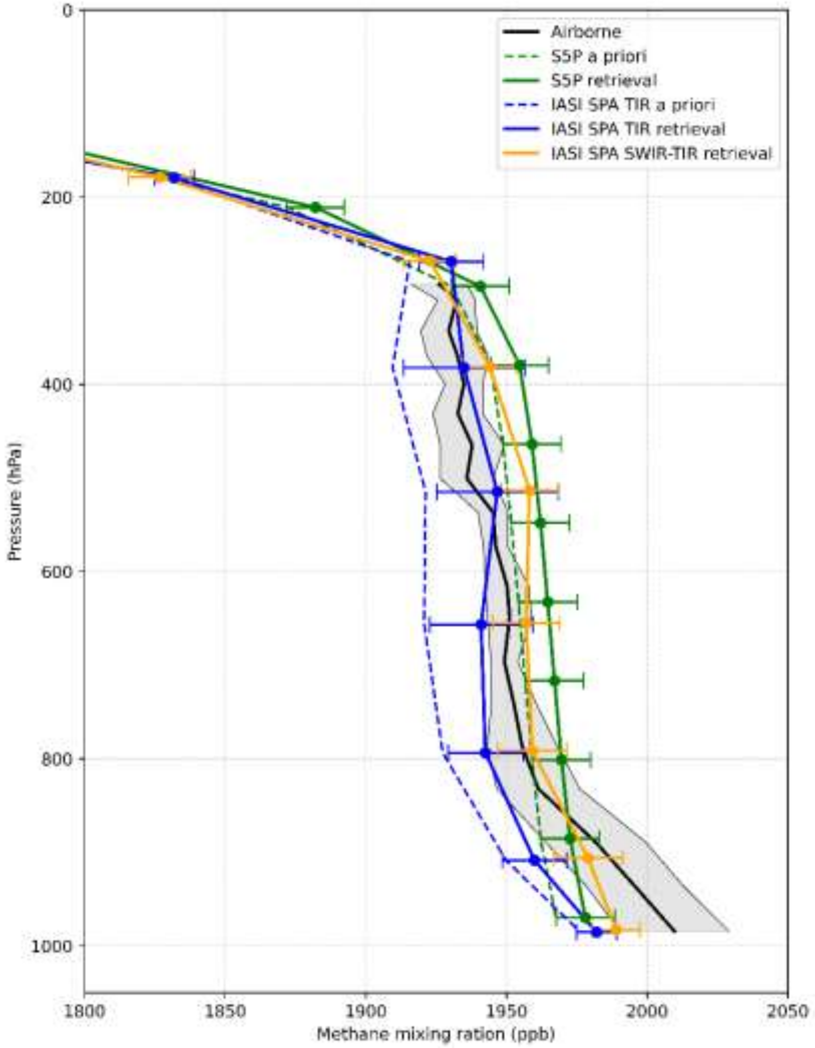


- The vertical profiles of IASI inversions are, in principle, already in good agreement with the in situ measurements of the airborne campaign, in both the lower and upper parts of the atmosphere.

- the vertical profiles obtained from the synergistic inversion of IASI and S5P are closer to the reference profiles in the lowermost part of the atmosphere, more constrained by the measurements (further from the a priori), and less dispersed.

Discussion

- Mean profiles on the L3 loop



- Although the retrieved products reproduce the vertical gradient in the lower layers, this is clearly constrained by the a priori profile used.

  - In the free troposphere (300-800hPa), where the IASI measurement provides the most information, we see an effect of the S5P measurement which tends to overestimate the solution of the inversion in synergy compared with the reference, which is not the case for the IASI inversion alone. This suggests to put more relative weight of IASI compared with that of S5P.

  - In the lower layers (between 800 and 1000 hPa), on the other hand, the synergistic inversion brings an improvement in the mean solution relative to the reference: the concentration in the lowest layers deviates from the a priori profile and approaches the reference value, and the mean value of concentrations in this vertical domain increases to approach that of the reference profile.

- Difficult in this case to assess the effect of synergy on the ability to restore a vertical gradient between 800 and 100 hPa, as this gradient is already present in the a priori CAMS profile used for inversion.

Conclusions and perspectives

The synergistic TIR+SWIR CH_4 retrieval combining L1 IASI spectra and L2 S5P vertical column density products shows **good performances** when compared with independent products and in situ reference measurements.

The analysis and validations are presented here for a dedicated region and period over Siberia. This **first exercise demonstrates** the **consistency of combining these complementary but different datasets** and the ability of this combination to **provide further information on the vertical profiles of CH_4.**

The TIR+SWIR retrieval processing is **ready to be applied over larger, representative datasets** in combination with correlative measurements. **An extensive validation is necessary for proposing a product**. The objective is to prepare a consolidated and validated retrieval processing ready for the combined **exploitation of data from the future IASI-NG and Sentinel 5** instruments onboard the Metop-SG platform.

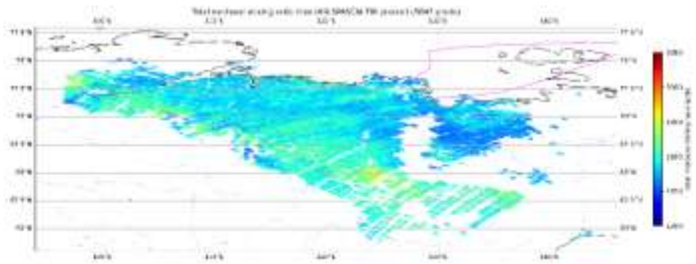
In addition, **needs for improvement in the retrieval process** have been identified, focusing on

1) the optimization of the weighted balance between TIR and SWIR measurement information,
2) the careful use of the a priori constraint
3) the consolidation of the observation operator used to constrain profile retrieval from S5P/TROPOMI SWIR product (removing contribution of a priori)

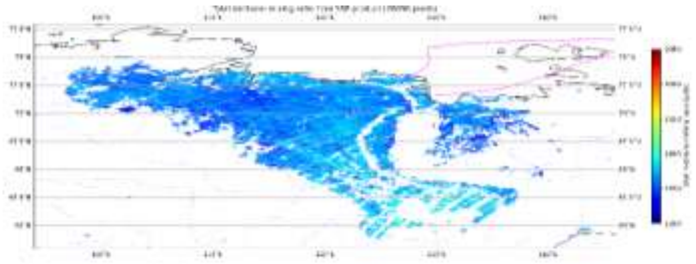
Perspectives : TIR+SWIR CH4 as an approach for product intercomparisons in Cal/Val IASI-NG ans Sentinel 5 on Metop SG

The synergistic TIR+SWIR CH_4 approach start by a careful statistical comparison of the IASI (IASI-NG) and S5P (S5) products
TIR+SWIR retrieval can be used as an objective frame for verifyng consistency (or identifying artefacts) at the IASI (IASI-NG) FOV scale

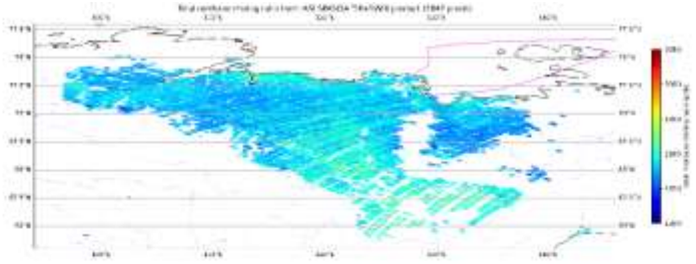
XCH_4 IASI TIR



XCH_4 S5P

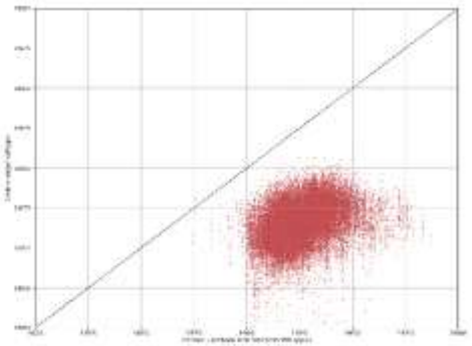


XCH_4 IASI TIR+SWIR (with bias correction)

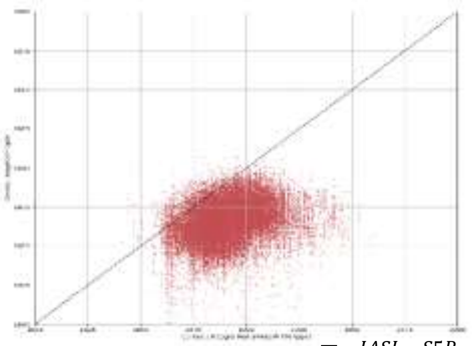


XCH_4 IASI TIR

S5P

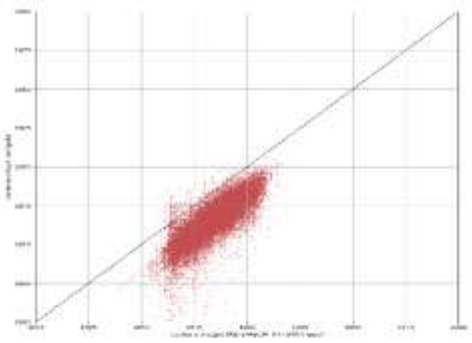


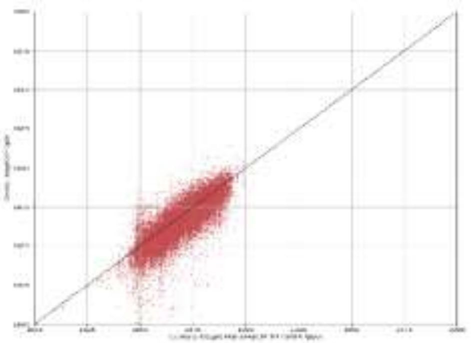
IASI TIR-SWIR $X_{CH_4}(IASI) = \frac{\sum x_i^{IASI}\ \delta p_i}{\sum \delta p_i}$



IASI TIR-SWIR $X_{CH_4} = \frac{\sum x_i^{IASI} w_i^{S5P} \delta p_i}{\sum w_i^{S5P} \delta p_i}$

XCH_4 IASI TIR+SWIR (with and without bias correction)





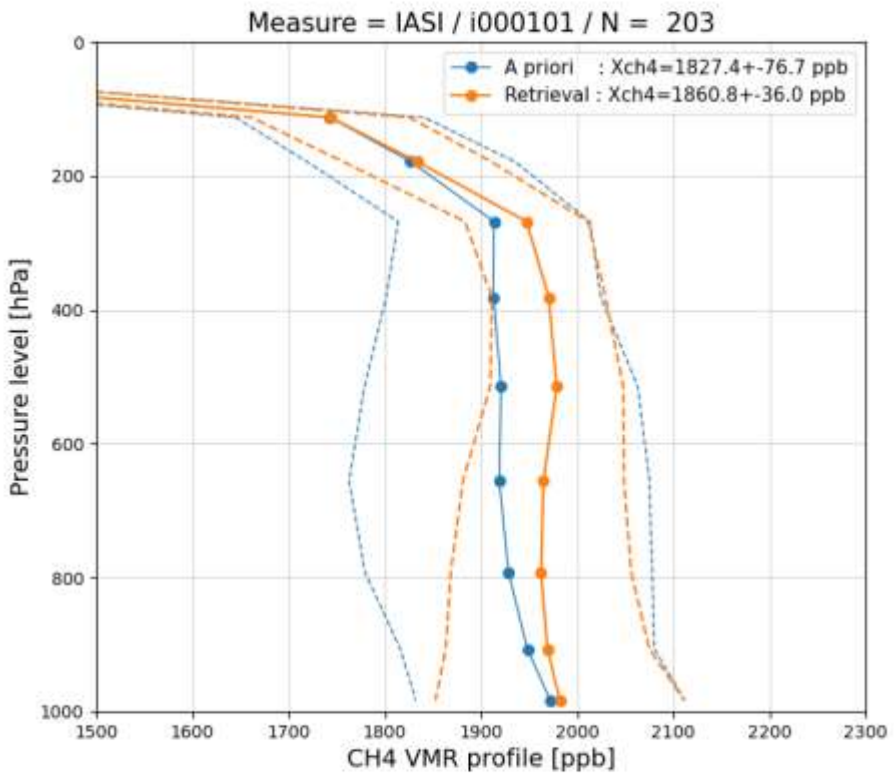
IASI TIR-SWIR $X_{CH_4} = \frac{\sum x_i^{IASI} w_i^{S5P} \delta p_i}{\sum w_i^{S5P} \delta p_i}$

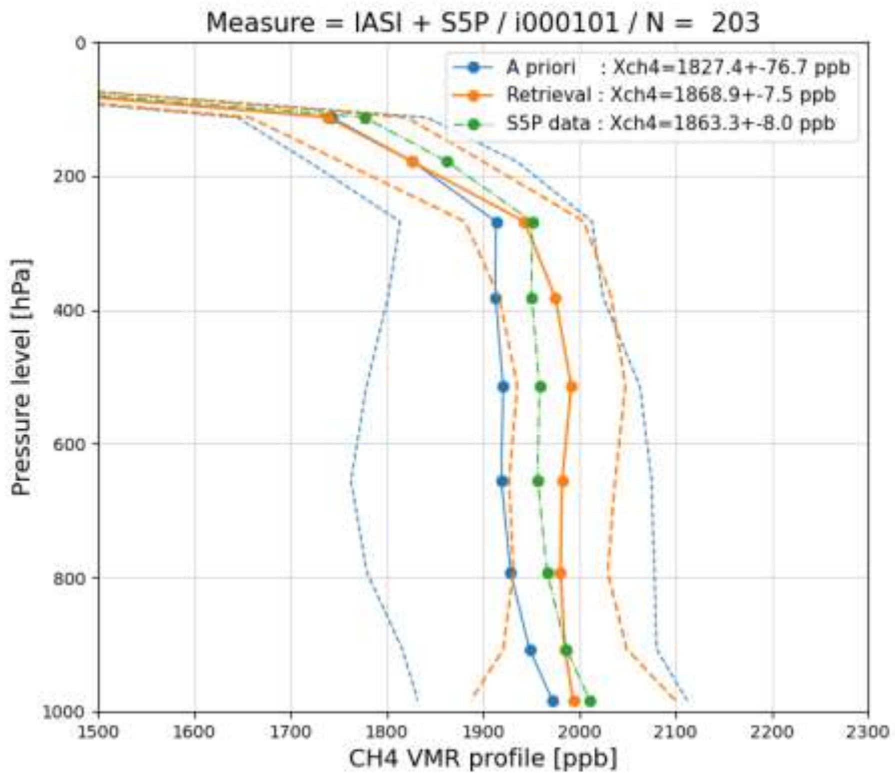
The comparison of the two products and the synergistic approach allow to analyse and quantify differences and biases in the two products, and to identify the parts of these differences that can be reduced through optimal combination (an improvement with respect to both products) and the part that can be associated to a persistent bias between the two products.

Thank you for your attention !

Inversion TIR+SWIR : premiers tests

- Profil : Illustration pour un IFOV en coïncidence *(Cloud Cover = 0% sur terre)*



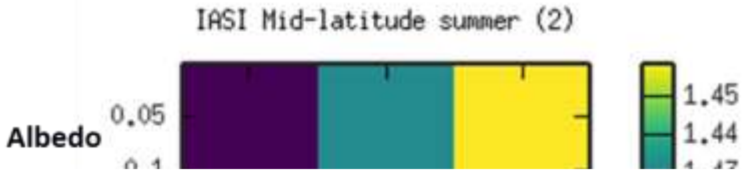


Theoretical analysis of TIR + SWIR combinations L1+L1, L1+L2

A SUPPR

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

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



Additional DOFS due to synergy varies between 0.0 and 1.0, most of the time above 0.5

- ➢ With respect to TROPOMI alone, largest added value of IASI is mostly for low albedo
- ➢ With respect to IASI alone, synergy is most favourable in case of negative or null thermal contrast, and depends on the atmosphere. The additional DOFS is most of the time above 0.7