Spectroscopy and forward model error improvement for CH4 retrieval in the TIR

Executive Summary

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ABSTRACT:

The goal of this activity was to identify and mitigate biases in satellite-based thermal infrared (TIR) measurements of methane. This would allow an improved synergistic use of shortwave infrared (SWIR) and TIR observations of methane by instrument on-board Metop-SG, to improve estimates of methane sources and sinks. Errors in forward model and retrieval schemes, spectroscopy and possible instrument biases were investigated, focussing on Metop IASI observations. The study provided an exhaustive review and quantification of uncertainties, and proposed mitigations. It was found that spectroscopic errors, and in particular insufficient representation of spectral line–mixing (LM), is the dominating error source at present. The implementation of state-of-the-art CH_4 line-mixing in the radiative transfer modelling, based on the most recent versions of HITRAN database and Trans' implementation of 1st order LM, has been achieved, and has been adapted to produce look-up-tables (LUTs) usable by radiative transfer and retrieval tools. In a case study, improvements of the retrieval of 1 month of methane profiles from IASI at a marine site with ground-based validation measurements were demonstrated using the new LM implementation. Spectroscopic measurements were also performed in the so-called ν_4 band, from 1190-1314 cm^{-1}, used for the IASI methane retrieval. Follow-on activities are recommended : 1) the impact of exploiting these newly measured spectroscopic data in retrieval tests shall be evaluated, and 2) new laboratory measurements are required to cover more extensively lines and multiplets of CH_4 in the domain 1200-1400 cm^{-1} in order to sample a wider variety of transition to better constrain the development of a full line-mixing model.

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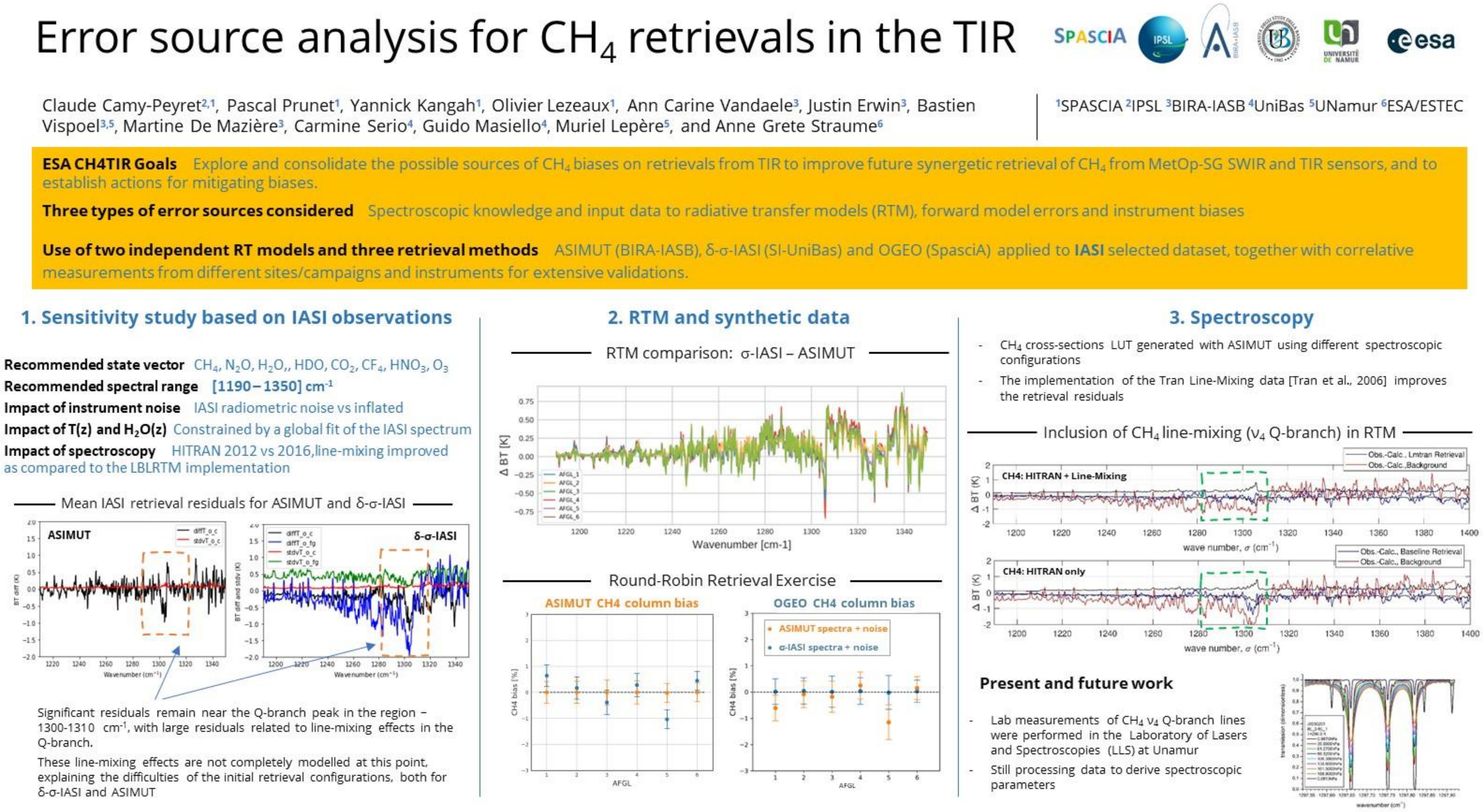

Error source analysis for CH_4 retrievals in the TIR

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ESA CH4TIR Goals Explore and consolidate the possible sources of CH_4 biases on retrievals from TIR to improve future synergetic retrieval of CH_4 from MetOp-SG SWIR and TIR sensors, and to establish actions for mitigating biases.

Three types of error sources considered Spectroscopic knowledge and input data to radiative transfer models (RTM), forward model errors and instrument biases

Use of two independent RT models and three retrieval methods ASIMUT (BIRA-IASB), δ-σ-IASI (SI-UniBas) and OGEO (SpasciA) applied to **IASI** selected dataset, together with correlative measurements from different sites/campaigns and instruments for extensive validations.

1. Sensitivity study based on IASI observations

Recommended state vector CH_4, N_2O, H_2O,, HDO, CO_2, CF_4, HNO_3, O_3
Recommended spectral range [1190 – 1350] cm^{-1}
Impact of instrument noise IASI radiometric noise vs inflated
Impact of T(z) and H_2O(z) Constrained by a global fit of the IASI spectrum
Impact of spectroscopy HITRAN 2012 vs 2016,line-mixing improved as compared to the LBLRTM implementation

Mean IASI retrieval residuals for ASIMUT and δ-σ-IASI

Significant residuals remain near the Q-branch peak in the region – 1300-1310 cm^{-1}, with large residuals related to line-mixing effects in the Q-branch.

These line-mixing effects are not completely modelled at this point, explaining the difficulties of the initial retrieval configurations, both for δ-σ-IASI and ASIMUT

2. RTM and synthetic data

RTM comparison: σ-IASI – ASIMUT

Round-Robin Retrieval Exercise

3. Spectroscopy

- CH_4 cross-sections LUT generated with ASIMUT using different spectroscopic configurations
- The implementation of the Tran Line-Mixing data [Tran et al., 2006] improves the retrieval residuals

Inclusion of CH_4 line-mixing (ν_4 Q-branch) in RTM

Present and future work

- Lab measurements of CH_4 ν_4 Q-branch lines were performed in the Laboratory of Lasers and Spectroscopies (LLS) at Unamur
- Still processing data to derive spectroscopic parameters

Figure 1 : Summary presentation of the CH4TIR study main achievements

Study objectives and approach

Atmospheric CH_4 is measured continuously from space-borne passive optical instruments, providing valuable information at global and regional scales not only for atmospheric monitoring but also 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). Nadir instruments in the TIR provide profile information, with typically a few pieces of information in the middle and upper troposphere. The synergistic exploitation of measurements in these two spectral domains, e.g. from the atmospheric composition sounders Sentinel-5 and IASI-NG on MetOp-SG, has a great potential for better understanding, quantifying and monitoring surface processes as well as sources and sinks of this species highly relevant to climate change.
The earlier ESA study SIROCCO revealed that CH_4 atmospheric concentration retrievals from TIR nadir sensors exhibits significant biases, as compared to independent observations, or when intercompared between different TIR and SWIR/TIR sensors products. Such biases hampers both use of TIR observations as well as the synergetic use of SWIR and TIR observations.

The aim of the CH4TIR study is to explore and consolidate the possible sources of the CH_4 biases published in the SIROCCO study and in the open literature in retrievals from TIR sensors, to establish necessary actions and perform the related work for mitigating biases.
This study distinguishes three types of error sources, which have been covered: **spectroscopic** knowledge and input data to radiative transfer models (RTM), **forward model** errors**,** and **instrument** biases.
We also carefully distinguished between the two terms "*error*" and "*uncertainty*", *error* designing the difference between the estimation and the truth, and *uncertainty* designing a quantitative evaluation of the expected error for any given spectral measurement and derived geophysical parameter.

The work has been based on the following activities.

- The use of three independent state-of-the-art RTM codes coupled to inversion algorithms base on the optimal estimation method (OEM): the ASIMUT forward model and retrieval scheme (**BIRA-IASB**), the δ-σ-IASI forward model and retrieval scheme (**SI-UniBas**), and the OGEO retrieval scheme (**SPASCIA/IPSL**). They have been tested against validation data and compared together, providing a well calibrated reference. They have been used independently for sensitivity tests and retrieval exercises, ensuring a robust analysis of the error sources and their impact on CH_4 biases.
- Retrievals and sensitivity tests on IASI actual measurements together with validation against an extensive independent datasets: ground-based FTIR, *in situ* and aircraft correlative datasets from NDAAC, HIPPO, and long-term series from Mauna Loa, Hawaii. Particularly the latter dataset was used extensively given its favourable conditions concerning collocated observations of the CH_4 vertical gradient in the lowermost part of the atmosphere, cloud screening and quasi-uniform surface conditions.
- An innovative work on spectroscopic issues: the CH_4 spectroscopy has been tested on selected spectral features from the residuals in the observed-calculated spectra. In parallel a dedicated small-scale laser spectroscopic measurement campaign of CH_4 line parameters has been performed in the 7.6 µm region (**Univ. Namur**).

Summary of achievements

From sensitivity analysis and examination of residuals provided by extensive CH_4 retrievals from real IASI data with two independent spectral inversion schemes, we have provided a comprehensive analysis of CH_4 TIR retrieval error sources (***Figure 1, part 1***). Solutions have been implemented to mitigate the impact of these error sources.

- We have derived consolidated recommendations for the optimal observation vector (spectral domain, observation vector uncertainty and covariance) and the optimal state vector (list of species to be considered and associated *a priori* information).
- We have identified the importance of determining the profiles T(p) and H_2O(p) through a global fit of the IASI spectra with a multivariate retrieval from a full-spectrum inversion (σ–δ-IASI approach).
- As the major remaining source of error we have identified line-mixing effects in the Q branch region of the ν_4 band of CH_4 around 1306 cm^{-1} as well as line-mixing in multiplets of the P branch at lower wavenumbers.
- The importance of reducing the residual peaks all over the spectral domain of interest for CH_4 has been highlighted for a better sensitivity to the target species CH_4.

From forward/inverse model intercomparisons (***Figure 1, part 2***), we have identified some critical aspects of the forward modelling (*radiative transfer vertical discretisation; a priori values/uncertainties or fixed parameter values/uncertainties (specific attention to the temperature profile);* H_2O *continuum; separate retrieval of* H_2O *and HDO; LUT parameterisation of optical depths*). We have improved forward modelling and demonstrated consistency of the two forward model radiances within the instrumental noise level in large parts of the modelled spectra. Remaining differences, in particular near 1306 cm^{-1}, are basically explained by line-mixing effects. This confirmed the priority to improve LM modelling.
An estimate of the forward model uncertainty as 3 times the IASI noise in the spectral domain specific for CH_4 retrievals (from 1190 cm^{-1} to 1350 cm^{-1}) has been initially proposed. But this is only a provisional measure to reduce biases on the retrieved methane product (avoiding overfitting RTM errors).

The improvement of LM modelling and spectroscopic parameters has been addressed in two parallel ways (***Figure 1, part 3***).

1) Laboratory measurements of line-by-line spectroscopic parameters of CH_4 in the Q branch of the ν_4 band (broadening and line-mixing coefficients) have been performed at University of Namur. The exploitation of these measurements is ongoing. Status and recommendation for required additional effort have been identified.
2) The careful implementation of state-of-the-art CH_4 line-mixing (LM) in the radiative transfer modelling, based on HITRAN and Trans' implementation of 1st order line-mixing, has been achieved by the BIRA-IASB team. It is now implemented in ASIMUT and has been adapted to produce look-up-tables (LUTs) usable by σ-δ-IASI (and possibly other RTMs). This is an original and valuable contribution of this project to account for LM effects in CH_4 retrieval.
   Improved spectroscopic modelling resulting from the BIRA CH_4-LM module shows a reduced absorption in the core of the ν_4 methane band. Its exploitation in the two forward models and retrieval schemes allows a better fit of the IASI spectrum (in particular for the methane Q-branch around 1305 cm^{-1}) and simultaneously improves methane retrievals. These improved results suggest that the LM implemented in LBLRTM v12.2, on which σ-IASI was based initially, does not correctly exploit Trans' implementation of 1st order line-mixing. The proper implementation of this parameterisation in the CH_4-LM module of ASIMUT allows to demonstrate a very positive added-value.

A two-step retrieval approach has been implemented, in order to mitigate the possible T(p) and H_2O(p) profile error/uncertainty sources in the ASIMUT retrieval (which exploits only the IASI spectral domain specific for CH_4 from 1190 cm^{-1} to 1350 cm^{-1}) by exploiting *(*as *a priori* for temperature and humidity profiles*)* the information obtained through a full IASI spectrum retrieval by σ–δ-IASI. This analyse confirms the importance of ensuring consistency between T(p), H_2O(p) and methane retrieval and demonstrate the impact of the choice of *a priori* data in the ASIMUT retrieval. Because of the practical difficulties for operational implementation of a full spectrum inversion scheme, additional studies are required to consolidate the proper choice (e.g., from NWP system or L2 IASI product) and exploitation of consistent T(p) and H2O(p) information in a methane retrieval exploiting the optimised spectral domain.

As an overall statement of the CH4TIR achievements it can be said that by accounting properly from spectroscopic modelling of line interference effects in the ν_4 band of CH_4, the full potential of powerful infrared sounders like IASI (and IASI-NG in the future) can be used to get more than the usual single piece of information (the column averaged XCH_4 mixing ratio), but provide information on the vertical distribution of methane with possibly two pieces of information (when thermal contrast is not detrimental). This combined with the information from the SWIR sounders (during the day) able to better constrain the total column will help to quantify surface sources from global satellite measurements specially when both sounders are on the same platform as expected for the IASI-NG and Sentinel5 instruments.

Recommendations

New laboratory measurements are required to cover more extensively lines and multiplets of CH_4 in the domain 1200-1400 cm^{-1} in order to sample a wider variety of transition to better constrain the line-mixing model. In addition, the development of a full line-mixing model (not just the 1st order Rozenkranz approximation) and a dedicated study of the possibility to speed up the computing process including full line-mixing is needed. It is strongly encouraged to mobilize the concerned European community and to define a programmatic approach for these new spectroscopic developments.