RAL SWIR-TIR L2-L2 CH4 Retrieval ATBD

ATBD

Prepared by

D. Knappett

R. Siddans

UKRI STFC RAL Space

Remote Sensing Group

Harwell Campus

Didcot, OX11 0QX

United Kingdom

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ACRONYMS

ATBD	Algorithm Theoretical Basis Document
CH_4	Methane
CO	Carbon Monoxide
ESA	European Space Agency
FM	Forward Model
IASI	Infrared Atmospheric Sounding Interferometer
IR	Infrared
L1	Level 1
L2	Level 2
Metop	Meteorological operational satellite
NCEO	National Centre for Earth Observation
OE	Optimal Estimation
RAL	Rutherford Appleton Laboratory
RSG	Remote Sensing Group
S5	Sentinel-5
S5P	Sentinel-5 Precursor
SWIR	Shortwave infrared
STFC	Science and Technology Facilities Council
TIR	Thermal infrared
TROPOMI	Tropospheric Monitoring Instrument
VMR	Volume mixing ratio

1 INTRODUCTION

1.1 PURPOSE

This is the algorithm theoretical basis document (ATBD) for version 1.0 of the Rutherford Appleton Laboratory (RAL) shortwave infrared and thermal infrared (SWIR-TIR) Level 2 – Level 2 (L2-L2) methane (CH_4) retrieval scheme. The purpose of this document is to provide a mathematical and physical description of the algorithm and describe its inputs. Details of the L2 output of the RAL SWIR-TIR L2-L2 retrieval scheme, and how to compare it with independent data, are described in the RAL SWIR-TIR L2 Methane v1.0 Product User Guide (RD-1).

2 REFERENCES

2.1 REFERENCE DOCUMENTS

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3 ALGORITHM DESCRIPTION

3.1 OVERVIEW

The RAL SWIR-TIR retrieval scheme for methane (CH_4) and carbon monoxide (CO) was developed by the RAL Remote Sensing Group via the ESA Living Planet Fellowship "Production of lower tropospheric methane and carbon monoxide distributions through combined use of ESA Sentinel-5 Precursor shortwave infrared and IASI/CrIS thermal infrared satellite data" (PROMCOM), which was jointly funded by ESA and the UK National Centre for Earth Observation (NCEO). The retrieval scheme combines existing Level 2 (L2) data products (either CH_4 or CO (sub-)column amounts) that have been retrieved from the SWIR and TIR spectral regions and is therefore described as a 'L2-L2' scheme. In the SWIR, the official Tropospheric Monitoring Instrument (TROPOMI) L2 products for CH_4 and CO are used. In the TIR, L2 data can be provided by retrievals based on either the Infrared Atmospheric Sounding Interferometer (IASI) or the Cross-Track Infrared Sounder (CrIS). To date, the TIR L2 component has been based on IASI for CH_4 and IASI or CrIS for CO.

The RAL SWIR-TIR L2-L2 retrieval scheme is based on the optimal estimation method (RD-2), which solves an otherwise under-constrained inverse problem by introducing prior information. By using the respective averaging kernels of the two input L2 retrieval products as the forward model, the reliance of the SWIR-TIR L2-L2 retrieval on the original *a priori* of either L2 input product is effectively removed and is replaced by a new, common prior.

3.2 SWIR-TIR RETRIEVAL METHOD

The SWIR-TIR L2-L2 combination is implemented by posing the problem as a linear retrieval in which we wish to optimally estimate a profile by combining the information contained in two existing L2 retrievals. The approach should work for a retrieval of any property linearly related to the profile e.g. (sub-)column amounts or mixing ratio profiles on a coarsely sampled vertical grid (provided the transformation to a fine grid is clearly defined). For the approach to work, it is assumed that averaging kernels are provided (or can be constructed) for all input retrievals, with respect to fine scale perturbations in the true profile (defined in the same units on the same finely resolved grid). First we describe the general approach, and the provide specifics of the SWIR-TIR methane retrieval.

We choose to represent the (output, optimised) profile in a flexible way on a fine vertical grid using N basis functions (this can be different from the way the input retrievals represent the profile):

$$\boldsymbol{r}(z) = o(z) + \sum_{i=1,N} x_i B_i(z),$$

Equation 1

where $o(z)$ is an "offset" profile (which can be considered as the new prior profile on the fine grid). $B(z)$ are a set of suitable basis functions (e.g. triangular functions representing linear interpolation from a coarse vertical grid, or principal components of the assumed profile variability). The N element vector $\boldsymbol{x}$ contains state vector elements to be retrieved.

This is written in the form of vectors and matrices, with vector $\boldsymbol{r}$ to describing the profile on a finely resolved vertical grid:

$$\boldsymbol{r} = \boldsymbol{o} + \boldsymbol{B}\boldsymbol{x},$$

Equation 2

where $\boldsymbol{B}$ is a matrix containing the N basis functions.

The optimal $\boldsymbol{x}$ (and hence $\boldsymbol{r}$) can be obtained using the input retrievals as the "measurements" for an OEM retrieval. These are contained in a measurement vector, $\boldsymbol{y}$. We can relate each to $\boldsymbol{r}$, using the averaging kernels as the forward model function:

$$y_j = \boldsymbol{A}_j(\boldsymbol{r} - \boldsymbol{r}_{\boldsymbol{aj}}) + a_j,$$

Equation 3

where index j represents a specific sub-column amount (from TIR or SWIR). $\boldsymbol{A}_j$ is the averaging kernel (vector) for this sub-column (from the TIR or SWIR retrieval), describing the derivative of the sub-column with respect to perturbations *on the fine grid*. $\boldsymbol{r}_{\boldsymbol{aj}}$ is the (finely resolved) prior profile used in the previous (input) retrieval and a_j is the corresponding prior sub-column amount.

Substituting for $\boldsymbol{r}$ gives

$$y_j = \boldsymbol{A}_j(\boldsymbol{o} + \boldsymbol{B}\boldsymbol{x} - \boldsymbol{r}_{\boldsymbol{aj}}) + a_j.$$

Equation 4

Using this (linear) forward model for $F(x)$, $\boldsymbol{x}$ can be estimated via minimisation of the usual cost function, χ^2, i.e.

$$\chi^2 = (\boldsymbol{x} - \boldsymbol{x}_{\boldsymbol{a}})^T \boldsymbol{S}_a^{-1}(\boldsymbol{x} - \boldsymbol{x}_a) + \big(\boldsymbol{y} - F(\boldsymbol{x})\big)^T \boldsymbol{S}_e^{-1}\big(\boldsymbol{y} - F(\boldsymbol{x})\big),$$

Equation 5

where the measurement covariance $\boldsymbol{S}_{\boldsymbol{e}}$ constrains the estimated error covariances of the (TIR+SWIR) sub-columns in $\boldsymbol{y}$. *A priori* covariance $\boldsymbol{S}_{\boldsymbol{a}}$ describes the estimated prior errors on the state vector (i.e. the basis function weights). In principle these are defined to represent realistic prior knowledge in the profile, though tuning to match the information content of the joint retrieval is likely to be needed in practise. The prior state itself, $\boldsymbol{x}_a$, is typically a vector of zeros, since the state describes increments to the offset profile, $\boldsymbol{o}$.

Since the forward model is linear, the solution which minimises the cost function is given by:

$$\hat{\boldsymbol{x}} = \boldsymbol{x}_{\boldsymbol{a}} + (\boldsymbol{K}^{\boldsymbol{T}}\boldsymbol{S}_{\boldsymbol{e}}^{-\boldsymbol{1}}\boldsymbol{K} + \boldsymbol{S}_{\boldsymbol{a}}^{-\boldsymbol{1}})^{-1}\boldsymbol{K}^T\boldsymbol{S}_{\boldsymbol{e}}^{-\boldsymbol{1}}(\boldsymbol{y} - F(\boldsymbol{x}_{\boldsymbol{a}})),$$

Equation 6

where weighting function matrix $\boldsymbol{K}$ is the derivative of the forward model with respect to the state parameters, i.e.

$$\boldsymbol{K} = \boldsymbol{A}\,\boldsymbol{B},$$

Equation 7

where $\boldsymbol{A}$ is the matrix containing the averaging kernels of the input retrieved amounts with respect to the fine scale profile (columns are $\boldsymbol{A_j}$ in Equation 4). Note that (assuming linearity), using the averaging kernel equation as the forward model operator, effectively removes the influence of the original retrievals prior constraint on the joint retrieval (this is effectively replaced by the new prior).

Given the solution state, it is trivial to compute the corresponding high-resolution version of the profile, $\boldsymbol{r}$ (Equation 2). Sub-column amounts for specific layers can then be calculated from that profile. This step can be carried out by matrix multiplication by matrix, $\boldsymbol{M}$, which contains the weights needed to integrated the profile to a set of sub-column amounts, such that

$$\boldsymbol{s} = \boldsymbol{M}\,\boldsymbol{r}.$$

Equation 8

Via the usual OEM equations, the total a posteriori errors on $\hat{\boldsymbol{x}}$ are described by covariance

$$\boldsymbol{S_x} = (\,\boldsymbol{K^T S_e^{-1} K} + \boldsymbol{S_a^{-1}}\,)^{-1}.$$

Equation 9

The (non-square) averaging kernel for $\hat{\boldsymbol{x}}$, giving derivatives of the solution with respect to *fine-scale* perturbations in the profile is given by

$$\boldsymbol{A_x} = \boldsymbol{S_x K^T S_e^{-1} A}.$$

Equation 10

($\boldsymbol{A}$, without subscript, is the derivative of the input retrievals with respect to fine-scale perturbations in the true profile).

The (square) averaging kernel for the output fine scale profile is:

$$\boldsymbol{A_r} = \boldsymbol{B A_x}.$$

Equation 11

The (non-square) averaging kernel for the derived sub-columns (with respect to fine scale perturbations in the profile) is:

$$\boldsymbol{A_s} = \boldsymbol{M A_r}.$$

Equation 12

Errors on the retrieval profile and sub-columns are described by covariances:

$$\boldsymbol{S_r} = \boldsymbol{B S_x B^T},$$

Equation 13

$$\boldsymbol{S_s} = (\boldsymbol{MB})\boldsymbol{S_x}(\boldsymbol{MB})^{\boldsymbol{T}}.$$

Equation 14

(The noise and smoothing error covariances can be similarly derived starting from the usual OEM expression for these matrices for the state vector $\hat{\boldsymbol{x}}$).

3.3 MEASUREMENTS

The dry-air column (or sub-column) averaged volume mixing ratio (VMR) is the vertically integrated number of molecules of methane (per unit surface area) divided by the similarly vertically integrated number of air molecules (excluding water vapour). In the following text we refer to this quantity simply as the column (or sub-column) averaged VMR. The column averaged VMR is also commonly referred to as 'XVMR'.

The measurement vector for the SWIR-TIR L2-L2 CH_4 retrieval scheme consists of 5 elements, as follows:

- SWIR column averaged CH_4 VMR
- TIR sub-column averaged CH_4 VMR for the 0-6 km, 6-12 km, 12-16km and 16-80km (i.e. top-of-atmosphere) layers.

In the SWIR, the input L2 product is the column averaged CH_4 VMR from TROPOMI, a nadir-viewing grating UV-VIS-NIR-SWIR spectrometer on board ESA's Sentinel 5 Precursor (S5P). TROPOMI covers the SWIR spectral region from 2.305-2.385 µm with a spectral resolution of 0.25 nm (RD-3) and has a 5.6 x 7.2 km footprint at nadir. The TROPOMI L2 CH_4 product is produced by the RemoTec-S5P retrieval scheme (RD-4), version 18_17.

In the TIR, the input L2 product is the RAL IASI Metop-B TIR Methane v2.0 dataset (RD-5; RD-6), referred to as Methane+ versions 1 (V1) data. IASI is a Fourier transform spectrometer onboard the Metop series of polar-orbiting satellites that covers the TIR spectral region discontinuously in three bands between 645-2760 cm^{-1} (15.5-3.63 µm). IASI observes four 12 km diameter footprints, arranged in a 2 x 2 matrix, simultaneously, with a distance of 17 km between the centre points of adjacent footprints at nadir (RD-7). The IASI L2 CH_4 product contains VMR profiles defined on fixed-pressure retrieval levels. For use in the SWIR-TIR L2-L2 retrieval we vertically integrate the VMR profile to produce two sub-column averaged VMRs (i.e. 0-6 km and 6-12 km, where the pressure-altitudes are in z*, and 0 km refers to the Earth's surface) and a column averaged VMR.

The Metop series of satellites have a daytime local equatorial crossing time of 09:30 on the *descending* node whereas S5P has a daytime local equatorial crossing time of 13:30 on the *ascending* node; IASI and TROPOMI measurements are therefore separated by at least 4 hours, with the separation often being larger (see Section 3.7 for details). By contrast, the Suomi-NPP satellite (carrying the TIR CrIS instrument) performs a very similar orbit to S5P, therefore TROPOMI and CrIS measurements are separated in time by around 5 minutes (RD-8; RD-9). The orbital differences between S5P and Metop would appear to point to the TROPOMI/CrIS combination being preferable to the TROPOMI/IASI combination, however analysis in the Methane+ project found that the information content of CrIS was reduced compared to that of IASI (due to its reduced spectral resolution) and larger biases were found for CrIS than IASI in comparisons to CAMS flux inversions. For this reason, the S5P+IASI combination was prioritised within the ESA Methane+ project. In the near future, IASI Next Generation (IASI-NG) and Sentinel 5 will be collocated on board the Metop second Generation (Metop-SG) satellite platform. A joint S5/IASI-NG L2-L2 retrieval based on precisely collocated SWIR and TIR measurements should then be possible.

The combined retrieval assumes that the input (sub)columns are not significantly biased. During the ESA Methane+ project, validation was carried out on both the SWIR and TIR product, revealing biases between the products of up to around 50ppb, depending on location and time of year. Within that project an initial SWIR-TIR product was produced in which the input (sub-) columns from both instruments were bias corrected using the zonal mean differences between the individual SWIR/TIR retrieval and CAMS flux inversion methane (v19r1), aggregated for each calendar month, considering the years 2018 and 2019 together. The analysis was performed only for scenes for co-located IASI and S5P, so that the bias correction was most relevant for scenes which would be used in the joint retrieval. The derived biases are illustrated in Figure 1. See the Methane+ TIR and SWIR-TIR validation report for more information on the comparisons to CAMS and validation of the resulting SWIR-TIR retrievals.

The monthly, zonal binned biases are bilinearly interpolated to the latitude and time of each IASI and S5P retrieval. Note that no bias correction is applied to the TIR sub-columns above 12km. Only the 0-6 and 6-12km sub-columns were bias corrected in this first application of the scheme.

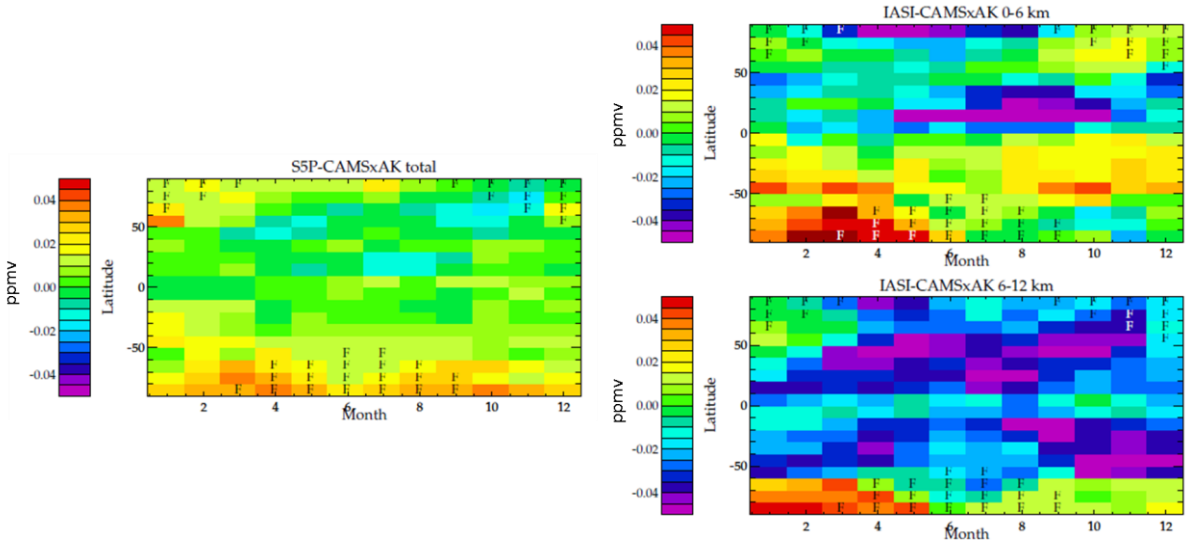

Figure 1: Illustration of the bias corrections applied to IASI and S5P sub-columns in the first application of the SWIR-TIR algorithm within the Methane+ project. Each panel shows zonal mean differences (for each month in 2018 and 2019 combined) between satellite (sub-)column averaged mixing ratio and CAMS (with averaging kernels applied), used to bias correct the (sub-)column amount before use in the joint SWIR-TIR retrieval, Left-hand panel shows S5P total column; upper-left hand panel shows IASI 0-6km sub-column; lower-left hand panel shows IASI 6-12km sub-column. The comparisons are only performed where there are pairs of S5P and IASI co-located retrievals on the same day. Grid cells where there are no such retrievals are filled by interpolation in latitude/month from neighbouring cells and indicated by the symbol ("F"). These are filled to ensure a well behaved interpolation of the binned values to the latitude and time of a given S5P/IASI retrieval (although points in the filled region will are rarely needed for this interpolation).

3.4 FINE GRID

The SWIR-TIR L2-L2 CH_4 retrieval scheme defines the fine vertical grid for the retrieval using the same hybrid sigma grid as used in the CAMS v19r1 flux inversions [RD-13,RD-14]. Using the hybrid sigma coordinate system, pressure levels used for a given profile are adjusted so that the lower atmospheric levels follow the surface pressure. The pressure levels an any individual profile are given by

$$\boldsymbol{p_{lev}} = \boldsymbol{A} + \boldsymbol{B}.p_{surf}$$

Equation 15

The constant vectors A and B are given in Table 1. The table also defines the pressure levels for a surface pressure of 1000hPa and the corresponding approximate altitude, according to

$$z^* = 16\left(3 - \log_{10}(p)\right)$$

Equation 16

A	B	Level pressure (for surface pressure 1000 hPa) / hPa	Approximate altitude z* / km
0	0	0	Top-of-atmosphere
0.9564	0	0.9564	48.31
2.985	0	2.985	40.4
7.132	0	7.132	34.35
16.81	0	16.81	28.39
39.6	0	39.6	22.44
60.18	0	60.18	19.53
73.07	0	73.07	18.18
87.65	7.58E-05	87.73	16.91
103.8	0.000461	104.2	15.71
120.8	0.001815	122.6	14.58
137.8	0.005081	142.8	13.52
153.8	0.01114	164.9	12.52
168.2	0.02068	188.9	11.58
180.5	0.03412	214.6	10.69
190.3	0.05169	242	9.86
197.6	0.07353	271.1	9.07
202.2	0.09967	301.9	8.322
204.3	0.13	334.3	7.613
203.8	0.1644	368.2	6.942
201	0.2025	403.4	6.307
195.8	0.2439	439.8	5.708
188.6	0.2883	477	5.144
179.6	0.3352	514.8	4.614
169	0.3839	552.9	4.118
144.1	0.4848	628.9	3.223
116.3	0.5862	702.5	2.454
88.02	0.6833	771.3	1.804
61.44	0.7716	833	1.269
38.51	0.8474	885.9	0.842
20.64	0.9079	928.5	0.5153
8.554	0.9518	960.4	0.2809
2.104	0.9797	981.8	0.1279
0.07368	0.994	994.1	0.04117
0	1	1000	0

Table 1: Hybrid sigma coordinates defining the fine grid (from CAMS flux inversion model).

3.5 STATE VECTOR

The state vector for the SWIR-TIR L2-L2 CH_4 retrieval scheme contains the dry-air volume mixing ratio CH_4 profile on 16 retrieval levels defined in hybrid sigma coordinates (so that the basis functions which relate the state to the fine grid are fixed). Retrieval levels corresponding to approximate altitude above the surface, z* = 0, 1, 2, 4, 6, 9, 12, 16, 20, 24, 28, 32, 36, 40, 50, and 60 km above the surface are chosen. The basis function are defined to perform linear interpolation in vmr as a function of pressure from this grid to the fine grid.

3.6 A PRIORI

The a priori state for the methane profile is defined used the same approach as the RAL TIR V2 TIR methane scheme (see RD-10), with adapted retrieval levels (as above) and modified prior covariance to all more freedom for the retrieval to (a) scale the whole profile (as in the RAL candidate V3 TIR scheme) and (b) adjust methane in the boundary layer. Details are given below.

3.6.1 DEFINITION OF A PRIORI STATE AND INITIAL ERROR COVARIANCE

As in the RAL TIR (V2 and V3), the *a priori* profiles are based on a combination of TOMCATand MACC greenhouse gas flux inversion fields: TOMCAT output based on the stratospheric assimilation (RD-12) of measurements by the ACE-FTS instrument was provided by the University of Leeds. These cover the period from 14 September 2008 to 9 September 2010, sampled every 6 hours at a horizontal resolution of approximately 2.8 degrees, with 60 vertical levels from the surface to 0.1 hPa. The zonal, annual mean of this dataset is determined using 5 degree latitude bins, interpolating profiles from the model levels onto a set of 65 fixed pressure levels (z^* values of 0 to 64 km in 1 km intervals). The corresponding standard deviations in the zonal mean are also determined (shown in the left hand panels of Figure 2). This is used to define the stratospheric distribution.

In the troposphere, a fixed vertical profile is assumed with latitude dependence taken from the annual zonal mean lower tropospheric mixing ratio of methane from the MACC greenhouse gas flux inversion data for 2009 ("v10-S1NOAA_ra", RD-14). For this purpose, the tropopause is assumed to correspond to the methane mixing ratio contour of 1.6 ppmv. The zonal mean methane values 3 km (in z* units) below this contour are set to that from the annual zonal mean MACC flux inversion. Linear interpolation is then used up to the 1.6 ppmv contour. The resulting mean methane field is shown in the left hand panel of Figure 2.

The profiles generated by this approach are there appropriate to methane levels in 2008/9. In other years, these profiles will be systematically biased due to the known methane trends, especially in recent years. The approach described in section 3.6.2 below is intended to address this, by including a strong vertically correlated error, which means that the prior constraint acts almost entirely on vertical structures, and the constraint on a scaling of the complete profile is very weak. In the joint retrieval, the column information from SWIR is very precise, so the fact that the prior profile is systematically biased to 2008/9 conditions is irrelevant to the results – the SWIR information will effectively scale the prior profile to match the observed column. It is possible that differing methane trends as a function of height (e.g. stratosphere vs troposphere) may lead some bias in the retrieval (due to the height resolved prior constraint), but this has not so far been observed to be a significant issue. Note that details of the choice of prior constraint are reflected in the retrieval averaging kernel, so have little impact on the use of data together with averaging kernels (e.g. in flux inversions).

The *a priori* profile and errors used for a specific IASI retrieval are initially derived from these annual mean and TOMCAT standard deviations as follows:

1. To avoid strong and very height-dependent constraint to the *a priori*, a minimum, relative error of 10% is imposed for the assumed prior errors. This is imposed in root-sum-square fashion as follows:

$$\Delta x_i = \sqrt{\Delta x_{T:i}^2 + (0.1\, x_{T:i})^2}$$

Equation 17

where Δx_i is the adjusted standard deviation at level *i* (for a given latitude bin); $\Delta x_{T:i}$ is the corresponding original TOMCAT derived standard deviation and $x_{T:i}$ is the TOMCAT/MACC derived mean value. The adjusted standard deviations are shown in the right hand panel of Figure 2. The choice of 10% relative error is somewhat empirical but, as can be seen in Figure 2, this corresponds to the model variability in the lower stratosphere (largely associated with dynamical variations about the zonal mean). Methane variability within the troposphere is smaller than this (of order few%) but we chose to maintain the 10% error within the troposphere to avoid over-constraining the retrieval to the prior, acknowledging the fact that plumes of methane from local sources can lead to departures from the zonal mean much larger than the model standard deviation.

2. The methane *a priori* profile and error is obtained by linearly interpolating the adjusted mean and standard-deviation fields to the latitude of the IASI observation, using the centre latitudes of each 5° zonal grid box. The values are also interpolated in altitude to the pressure levels defined in section 3.5.

Diagonal elements of the *a priori* covariance between levels *i* and *j*, C_{ij}, are set to the square of the adjusted standard deviations. Off diagonal elements are defined assuming a Gaussian correlation in the vertical with full-width half-maximum 6 km (in z^* units). This covariance matrix is illustrated in Figure 3 (in the panel labelled "TOMCLI").

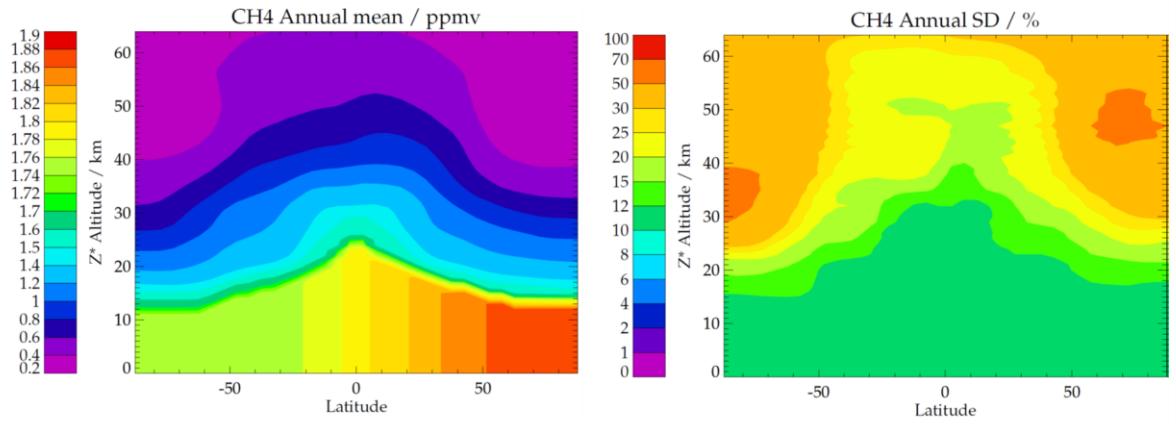

Figure 2: Illustration of methane *a priori* profiles and errors, derived from the TOMCAT and MACC fields. Left-hand panel shows 5 degree multi-annual zonal mean, used as the *a priori* profile. Right-hand panel shows the assumed standard deviation (SD), used as the *a priori* error.

3.6.2 MODIFICATION OF THE A PRIORI COVARIANCE

Following the approach of the RAL TIR candidate V3 scheme, an additional covariance is added to that defined above, to gives the retrieval freedom to scale the entire profile, while retaining the relative covariance between the levels in the profile. This is accomplished by modifying prior covariance for as follows:

$$C'_{i:j} = C_{i:j} + x_{T:i}.x_{T:j}$$

Equation 18

I.e. a fully correlated covariance representing 100% relative uncertainty in the profile is added to the covariance matrix. This means that the prior constraint on the retrieved total column is very weak. In the case that only a total column observation (from SWIR) is provided as measurement to the joint retrieval, then the retrieval will almost exclusively scale the prior profile such that the retrieved total column matches the measured (SWIR) value.

This covariance matrix is illustrated in Figure 3 (in the panel labelled “TOMCLI_TC”).

To allow the retrieval to independently modify the methane profile in the boundary layer, an additional error of 0.3ppmv is assumed to apply to the 0 and 1km retrieval levels, and this is assumed to be fully correlated between those two levels. I.e. a value of 0.3*0.3=0.09 ppmv^2 is added to the added to elements $C'_{i:j}$ for i=0 to 1 and j=0,1 (the diagonal elements and also the cross terms).

This final covariance matrix is used in the joint SWIR-TIR retrieval and is also illustrated in Figure 3 (in the panel labelled “TOMCLI_TCBL”).

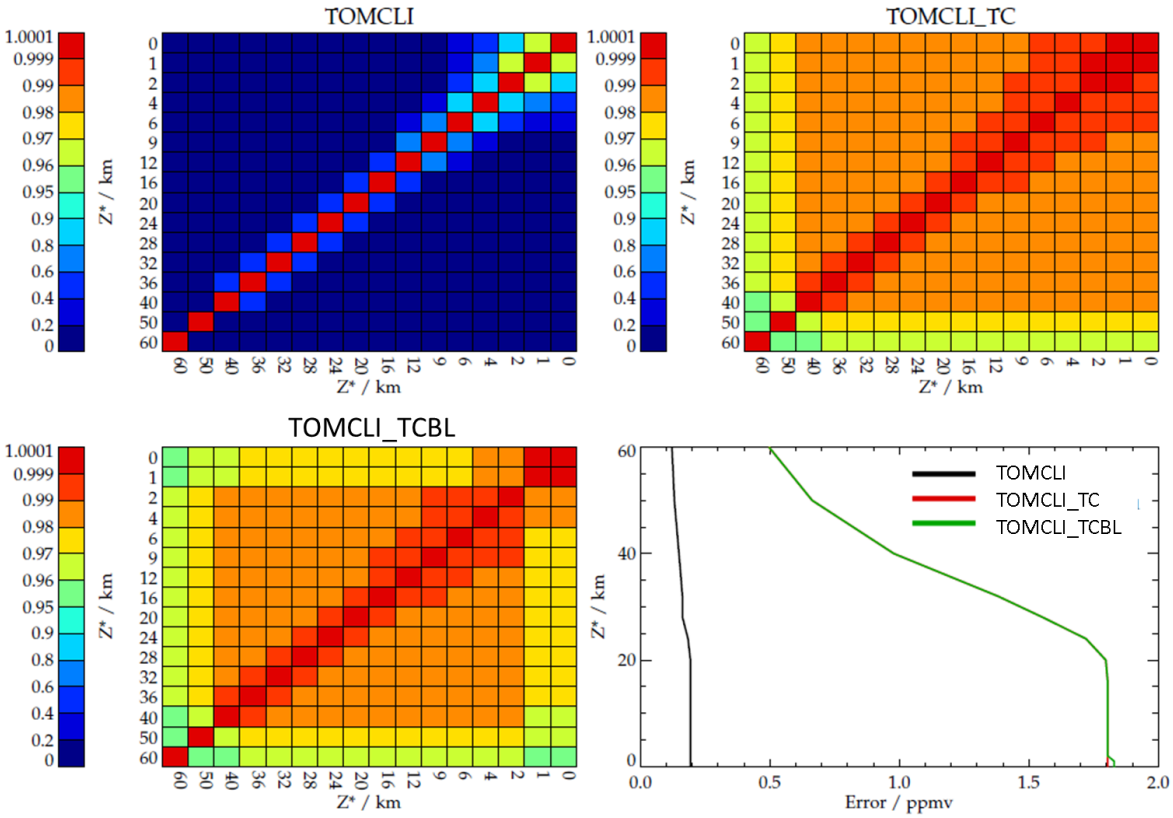

Figure 3: Stages in the construction of the *a priori* covariance used in the joint retrieval. Top left hand panel shows ("TOMCLI") shows the original correlation matrix based on TOMCAT variability and assuming a 6km vertical correlation length. Top-right hand panel ("TOMCLI_TC") shows the matrix after adding a vertically fully correlated matrix to represent scaling of the whole profile. Bottom-left panel ("TOMCLI_TCBL") shows the matrix after adding a further term to represent independent variations in the boundary layer. The bottom-right hand panel shows the square-root diagonal elements of each covariance matrix (i.e. the *a priori* errors).

3.7 SWIR-TIR SCENE MATCHING

The SWIR-TIR L2-L2 CH_4 combination is performed at the locations of SWIR (TROPOMI) soundings to ensure that small-scale features observed by TROPOMI (5.6 x 7.2 km resolution) are not missed by the lower resolution sampling of IASI (12 km). Spatial coverage of the combined retrieval is therefore determined predominantly by TROPOMI for which stringent cloud criteria are applied in the production of L2 output, although it can be further limited by other quality control indicators for TROPOMI and IASI individually and in combination. A combined SWIR-TIR retrieval L2 output file is produced for each input TROPOMI L2 file.

The TIR data for each TROPOMI scene is taken from the closest IASI L2 scene, within a maximum distance of 30 km between the centres of the TROPOMI and IASI footprints. S5P (TROPOMI) and Metop-B (IASI) orbit tracks cross because they have daytime ascending and descending nodes respectively. Metop-B orbits within +/- 6 hours of the S5P orbit start time are considered. Where swaths overlap (at mid-high latitudes), data from the closest orbit in time to S5P is selected. Consequently, scenes in a S5P orbit will match IASI scenes from several Metop-B orbits and the difference in observation time between IASI and TROPOMI retrievals will vary considerably along-track. Both the spatial and temporal differences between the SWIR and TIR measurements are stored in the SWIR-TIR L2-L2 CH_4 retrieval L2 output file.

It should be noted that only scenes where a SWIR and matching TIR retrieval exist are included in the output file. Since most cloud-free scenes are processed by the TIR retrieval, and IASI has near global coverage, the combined coverage remains comparable to that of S5P although it is, by definition, reduced (for some S5P scenes no matching TIR retrieval is found).

The same TIR retrieval will match multiple S5P scenes. For example, considering ideal cloud-free, near-nadir observing conditions, IASI footprints are ~12 km diameter, spaced every ~25 km along and across-track; each IASI scene will therefore be matched with all the (spatially contiguous) ~5.6 x 7.2 km S5P scenes within the corresponding ~25 x 25 km area.

4 USE OF AVERAGING KERNELS

Retrieved sub-columns should be compared to independent data (e.g. model data) by applying the averaging kernels as follows:

$$C_{Mxl} = c_a + \boldsymbol{A_f}(\boldsymbol{x_f} - \boldsymbol{a_f}),$$

Equation 19

where:

C_{Mxl} is the expected retrieved methane sub-column corresponding to the given model methane profile

c_a is the a priori methane sub-column for a given retrieved methane profile from the combined scheme

$\boldsymbol{A_f}$ is the averaging kernel on a fine grid for the given sub-column amount

$\boldsymbol{x_f}$ is the model profile interpolated onto the fine grid on which the averaging kernels are defined

$\boldsymbol{a_f}$ is the retrieval a priori profile also defined on the fine grid. This can be obtain using the a priori state vector together with the basis functions, which map from the state vector to the fine grid, using Equation 2

Further information regarding the use of the products is provided in the SWIR-TIR product user guide [RD-1].