SCIAMACHY 1b to 2 Off-line Processing
Instructions for the Usage
Of the Level 2 Product Limb MDS

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1 Introduction

1.1 Purpose and Scope of Document

SCIAMACHY is a joint project of Germany, The Netherlands and Belgium for atmospheric measurements. SCIAMACHY has been selected by the European Space Agency (ESA) for inclusion in the list of instruments for Earth observation research for the ENVISAT-1 polar platform, to be launched in 1999. The SCIAMACHY programme is currently in progress under the supervision of the SCIAMACHY science team (SSAG), headed by the Principal Investigators Professor J. P. Burrows (University of Bremen, Germany), Dr. A. Goede (SRON, The Netherlands) and Dr. C. Muller (BIRA, Belgium).

The Remote Sensing Technology Institute (IMF) which has been founded in 1999 as split of German Remote Sensing Data Centre (DFD) and other DLR institutes, plays a major role in the design, implementation and operation of the SCIAMACHY ground processors (SGPs) which are part of the ENVISAT payload data segment (PDS), as described in [A1]. The present document is part of the technical documentation provided by DLR for the design and implementation of the SCIAMACHY Level 1b-2 Off-line Processor (SGP L12 OL). The funding for these tasks is available through the *Deutsche Agentur für Raumfahrtangelegenheiten* (DARA) in Bonn as part of the ENVISAT phase C/D grant.

This document shall provide users of the Level 2 product who are interested to use the products retrieved from Limb observation measurements, information about the usage of the entries to the product. This shall also support the validation of the product.

1.2 Documents

1.2.1 Applicable Documents

Following documents are applicable for the technical background

[A1] ENVISAT-1 Ground Segment Concept, ESA/PB-EO(94)75, Issue 5, 20 September 1994

[A2] ESA Software Engineering Standards, ESA PSS-05-0, Issue 2, Feb. 1991

[A3] ENVISAT Product Specification Volume 15

[A4] ENVISAT SCIAMACHY Level 1b-2 Off-line Processing: Input/Output Data Definition, Issue 4 Rev. G, 15 March 2006

1.3 Abbreviations and Acronyms

A list of abbreviations and acronyms which are used throughout this document is given below:

ADD	Architectural Design Document
ADS	Annotation Data Set
AO	Announcement of Opportunity
CFI	Customer Furnished Items
DARA	Deutsche Agentur für Raumfahrtangelegenheiten
DFD	Deutsches Fernerkundungsdatenzentrum
DLR	Deutsches Zentrum für Luft- und Raumfahrt e.V.
D-PAC	German Processing and Archiving Centre
DSD	Data Set Descriptor
ENVISAT	Environmental Satellite
ESA	European Space Agency
ESRIN	European Space Research Institute
ESTEC	European Space Centre of Technology
GADS	Global Annotation Data Set
IMF	Institut für Methodik der Fernerkundung, DLR e.V.
IODD	Input/Output Data Definition Document
IPF	Instrument Processing Facility
MDS	Measurement Data Set
MJD	Modified Julian Day
MPH	Main Product Header
NRT	Near Real Time
PAC	Processing and Archiving Centre
PDS	Payload Data Segment
SCIAMACHY	Scanning Imaging Absorption Spectrometer for Atmospheric Chartography
SGP	SCIAMACHY Ground Processor
SPH	Specific Product Header
SSAG	SCIAMACHY Scientific Advisory Group
TOA	Top of Atmosphere
UV	Ultra-Violet
VIS	visible
VMR	Volume Mixing Ratio

1.4 Document Overview

The present document provides information about:

- Purpose and Scope of the document which includes the reference listings and the abbreviation list,
- The second section provides an overview about the entries of the Limb MDS of the SCIAMACHY Level 2 OL product,
- Some entries are discussed in more detail in the third section, and
- The document is finalized with some approaches for the conversion between different representations of profile products.

2 Definition of Entries in Limb MDS

To the users' convenience we recall the entry definitions as they are provided in the IODD and the Product Specification Document. Before serving any entry with comments, the pure format is described as it is specified. For that we provide the units and data types which are in usage.

An additional section will then highlight and comment some entries in more detail.

2.1 Units and data types

2.1.1 Unit Convention

For units the usual standard is used. More detailed specification can be found elsewhere [A4].

2.1.2 Data Types

Following basic data types are used and given in short notation:

Notation	Description	Length in Bytes
b	binary field	1
do	double (8-byte floating point number)	8
fl	float (4-byte floating point number)	4
sc	signed character (1-byte integer)	1
sl	signed long (4-byte integer)	4
ss	sigend short (2-byte integer)	2
tx	text field	1
uc	unsigned character (1-byte integer)	1
ul	unsigned long (4-byte integer)	4
us	unsigned short (2-byte integer)	2

The byte ordering of integer is such that the least significant byte is on the lower address.
The IEEE 754-1985 norm is the chosen standard for storing real numbers.

In addition, compound data types are used:

Notation	Description	Length in Bytes
Coord	Geographical coordinate (ISO 6709)	8
LayerRec	Limb profile layer record	16
MeasGrid	Measurement grid record	33
MJD	Modified Julian Day	12
StateVec	State vector record	12

From those all are used except "Coord" since the geographical coordinates are provided in the ADS for Limb geometry.

Limb Profile Layer Record (LayerRec)

No	Name	Description	Unit	Type
1	TANGVMR	Tangent layer volume mixing ratio	ppV	fl

No	Name	Description	Unit	Type
2	ERRTANGVMR	Error on TANGVMR	%	fl
3	VERTCOL	Vertical column density per layer	molecule/cm^2	fl
4	ERRVERTCOL	Error on VERTCOL	%	fl

Measurement Grid Record (MeasGrid)

No	Name	Description	Unit	Type
1	STARTTIME	Start time of measurement at that specific layer	-	MJD
2	TANGH	Mean tangent height of measurement	km	fl
3	TANGP	Pressure at tangent height	hPa	fl
4	TANGT	Temperature at tangent height	K	fl
5	NUM_WIN	Number of fitting windows	-	uc
6	WINMIN	Minimum wavelength of fitting windows	nm	fl
7	WINMAX	Maximum wavelength of fitting windows	nm	fl

Note that all information provided in this compound data type are related to the measurement grid which is in the most cases not identical to the retrieval grid.

Modified Julian Day (MJD)

No	Name	Description	Unit	Type
1	DAYS	Number of elapsed days since 1.1.2000 00:00 hour	day	sl
2	SECONDS	Seconds elapsed since the beginning of the day	s	ul
3	USECS	Microseconds elapsed since the beginning of the day	s	ul

State Vector (StateVec)

No	Name	Description	Unit	Type
1	VALUE	Value of the State vector entry	-	fl
2	ERROR	Error on VALUE	%	fl
3	TYPE	Type of VALUE (Annotation)	-	b

2.2 Limb MDS Entries Summary

The total Limb MDS is summarized in the following table.

No	Name	Description	Unit	Typ	Size
1	STARTTIME	Start time of profile record	-	MJD	
2	DSRLEN	Data set record length	-	ul	
3	QUALITY	Quality indicator (-1 if DSR empty)	-	sc	
4	INTTIME	Integration time for each individual step in the measurement grid	1/16 s	us	

No	Name	Description	Unit	Typ	Size
5	METHOD	Retrieval method	-	uc	
6	REFH	Height of the reference pressure	km	fl	
7	REFP	Reference pressure of hydrostatic equilibrium	hPa	fl	
8	REFPSRC	Reference pressure source	-	uc	
9	NUM_RLEVEL	Number of retrieval levels	-	uc	n_{main}
10	NUM_MLEVEL	Number of measurement levels	-	uc	n_{meas}
11	NUM_SPECIES	Number of fitted main gas species	-	uc	n1
12	NUM_CLOSURE	Number of fitted closure parameters	-	uc	n2
13	NUM_OTHER	Number of fitted other parameters	-	uc	n_3
14	NUM_SCALE	Number of fitted scaling parameters for auxiliary gases	-	uc	n_4
15	TANGH	Tangent height at the lower layer boundary	km	array of fl	n_{main}
16	TANGP	Tangent layer pressure at the lower layer boundary	hPa	array of fl	n_{main}
17	TANGT	Tangent layer temperature	K	array of fl	n_{main}
18	MAINREC	Main species which have been fitted on the coarse forward model grid	-	LayerRec	$n_{main}*n_1$
19	SCALEDREC	Scaled profiles which have been used for the fit on the coarse forward model grid	-	LayerRec	$n_{main}*n_4$
20	MGRID	Measurement Grid (see below)	-	MeasGrid	n_{meas}
21	STVEC_SIZE	State vector size (n_{stvec})	-	us	
22	STATEVEC	State vector (see below)	-	StateVec	n_{stvec}
23	CMATRIXSIZE	Size of correlation matrix	-	us	
24	CORRMATRIX	Correlation matrix of the fit	-	fl	
25	RMS	RMS of the fit	-	fl	
26	CHI2	χ^2 of the fit	-	fl	
27	GOODNESS	Goodness of the fit	-	fl	
28	ITERATION	Number of iterations	-	us	
29	SUMMARY	Measurement summary	-	us	
30	CRITERIA	Convergence criteria	-	b	
31	RESSIZE	Residuals size (n_{res})	-	us	
32	RESIDUALS	Iteration step state vector residuals	-	array of fl	n_{res}
33	NUM_ADDDIAG	Number of additional diagnostics entries	-	us	n_{add}
34	ADDDIAG	Additional diagnostics	-	array of fl	

Following notes have to be taken into account:

1. The product format has been defined with respect to usability to different retrieval methods and forward models in advance. From this not every entry serves identically for all methods applied in its meaning. In general, the selected method and the chosen retrieval grid finally provide the most appropriate representation of the results.
2. There are entries based on compound data types, e.g. arrays of compound data types.
3. The tangent height, pressure and temperature at tangent height are all provided on two different grids: the measurement grid (entry #20) and the retrieval grid (entries # 15, 16, and 17).
4. The last entry "ADDDIAG" contains in one array of floats some information about the retrieval. The content of "ADDDIAG" has been extended with version 3.0 of the SCIAMACHY Level 1b-2 OL data processor to provide data users some more detailed and complete information. The entry "ADDDIAG" is split into following details:

No	Description	Size	Last Position
1	Degree of freedom of retrieval	1	1
2	Information content	1	2
3	Diagonal elements of averaging kernel in vertical columns (partial columns)	n_{stvec}	$n_{stvec}+2$
4	Number density per layer of each main gas	n_1*n_{main}	$n_1*n_{main}+n_{stvec}+2$
5	Initial number density per layer of each main gas	$n_1* n_{main}$	$2*n_1*n_{main}+n_{stvec}+2$
6	Conversion factors to VMR per layer	n_{main}	$n_{main}+2*n_1*n_{main}+n_{stvec}+2$
7	Conversion factors to number density per layer	n_{main}	$2*n_{main}+2*n_1*n_{main}+n_{stvec}+2$
8	Averaging kernel for each main gas	$n_1*n_{main}*n_{main}$	$n_1*n_{main}*n_{main}+2*n_{main}+2*n_1*n_{main}+n_{stvec}+2$

3 Comments on Limb MDS

In order to provide some more detailed information for the data user of the Limb MDS, we present a short sub-section with some definitions which will be followed by comments to some MDS entries. Finally, we provide some more details about the computation loops which are behind the entry "ADDDIAG".

3.1 Quantity Definitions Used in Limb MDS

We define

- Number of elements of the retrieval grid: n_{main}
  (= number of profile entries and number of layers)
- State vector: x
- Element index per layer: $k=1,n_{main}$
- State vector elements assigned to partial columns per layer: $x_k,\ k=1,n_{main}$
  (Vertical columns per layer = partial columns per layer)
- Retrieval grid:
  - Ordering: top to down
  - Top of atmosphere is fixed to 100 km and used for the height grid
  - Information at TOA is used for height and pressure grid
  - Height at the lower boundary of each layer k: z_k
  - Pressure at the lower boundary of each layer k: p_k
  - Altitude grid element: $\Delta z_k = z_{k-1} - z_k$ with z_0 = 100 km
  - Pressure grid element: $\Delta p_k = p_k - p_{k-1}$
  - Pressure is read from climatology with p_0 at top of atmosphere
- Number density per layer: n with $n_k,\ k=1,n_{main}$
- Volume mixing ratio per layer: vmr with $vmr_k,\ k=1,n_{main}$

Since it is very often desirable to represent the retrieved profile in number density or volume mixing ratio, the relations with respect to the chosen state vector representation (partial columns per layer) are given in the following. Note that the conversion is related to quantities which describe the result for a given profile layer. Additionally, note that the information provided for pressure and height is implicitly extended by the entries at TOA which are not given in the product.

The number density at layer k can be derived from the state vector by

$$n_k = s_k^{nd} x_k = \frac{c_k^{nd}}{\Delta z_k} x_k$$

Here, s_k^{nd} is a scaling factor which can be expressed by the difference of the altitudes at the boundaries of the layer k

$$\Delta z_k = z_{k-1} - z_k$$

and the constant c_k^{nd}.

In analogy, the VMR at layer k is given by

$$vmr_k = s_k^{vmr} x_k = \frac{c_k^{vmr}}{\Delta p_k} x_k$$

There, the scaling factor s_k^{vmr} is expressed as the difference of the pressures at the boundaries of layer *k*

$$\Delta p_k = p_k - p_{k-1}$$

and the constant c_k^{VMR}.

The conversion between the State vector representation in partial columns and number density resp. VMR can also be written in matrix representation. Then, we have

$$n = \overline{S}^{nd} x \quad \text{and} \quad vmr = \overline{S}^{vmr} x$$

with $\overline{S}^{nd}$ and $\overline{S}^{vmr}$ being diagonal matrices, i.e. $\overline{S}_{ij}^{nd} = s_i^{nd} \delta_{ij}$ and $\overline{S}^{vmr}{}_{ij} = s_i^{vmr} \delta_{ij}$.

The conversion can also be applied to the representation of the covariance matrix, the correlation matrix, the relative error, and finally the averaging kernel.

Covariance Matrix

The covariance matrix $\overline{C}^x$ for the given state vector is written by

$$\overline{C}^x = E\left[xx^T\right]$$

where E is the expected value operator. The covariance matrix can be then converted into number density representation by

$$\overline{C}^{nd} = \overline{S}^{nd} \overline{C}_x \overline{S}^{nd}$$

and into VMR representation by

$$\overline{C}^{vmr} = \overline{S}^{vmr} \overline{C}_x \overline{S}^{vmr}.$$

Explicitly, the entries of $\overline{C}^{nd}$ and $\overline{C}^{vmr}$ can be expressed to

$$\overline{C}_{ij}^{nd} = s_i^{nd} C_{ij}^x s_j^{nd}$$

and

$$\overline{C}_{ij}^{vmr} = s_i^{vmr} C_{ij}^x s_j^{vmr},$$

respectively.

Relative Error

The relative error ε_i at the solution is defined by

$$\varepsilon_i = \frac{\sqrt{C_{ii}^x}}{x_i} \times 100 = \frac{\sqrt{C_{ii}^{nd}}}{n_i} \times 100 = \frac{\sqrt{C_{ii}^{vmr}}}{vmr_i} \times 100.$$

Correlation Matrix

The off-diagonal elements of the correlation matrix of the fit are given by

$$\rho_{ij} = \frac{C_{ij}^x}{\sqrt{C_{ii}^x}\sqrt{C_{jj}^x}} = \frac{C_{ij}^{nd}}{\sqrt{C_{ii}^{nd}}\sqrt{C_{jj}^{nd}}} = \frac{C_{ij}^{vmr}}{\sqrt{C_{ii}^{vmr}}\sqrt{C_{jj}^{vmr}}}$$

where $i\,j = 1, n_{main}$ and $i \neq j$.

Averaging Kernel

If $\hat{x}$ represents the "true" profile in partial columns per layer, then the averaging kernel is defined by

$$\overline{A}_{ij}^{x} = \frac{\partial \hat{x}_i}{\partial x_j}.$$

The averaging kernels for the number density and VMR are then given by

$$\overline{A}_{ij}^{nd} = \frac{\partial \hat{n}_i}{\partial n_j} = \frac{s_i^{nd}}{s_j^{nd}} \overline{A}_{ij}^{x} = \frac{s_i^{nd}}{s_j^{nd}} \frac{\partial \hat{x}_i}{\partial x_j}$$

and

$$\overline{A}_{ij}^{vmr} = \frac{\partial \hat{vmr}_i}{\partial vmr_j} = \frac{s_i^{vmr}}{s_j^{vmr}} \overline{A}_{ij}^{x} = \frac{s_i^{vmr}}{s_j^{vmr}} \frac{\partial \hat{x}_i}{\partial x_j},$$

respectively.

3.2 Comments on Limb MDS Entries

For a better understanding, some explanations are provided for a selection of Limb MDS entries.

3.2.1 Entry # 5: Retrieval Method

An one-character letter provides the user the information about the applied retrieval method.

Those are

Retrieval Method	Value assignment in entry 5
Optimal Estimation	
General Least Squares	
Tikhonov Regularization	
IRGN	

3.2.2 Entry # 11: Number of fitted main gas species

Usually, the retrieval in one application is dedicated to derive the profile information for a specific species. Since contribution of other constituents can be found in the spectra, those are taken into account in the retrieval scheme. In principle, there are two opportunities to include another species in the retrieval:

1. apply an a priori profile of a minor trace gas in the retrieval scheme and include it by scaling through a single factor (see entry #14)
2. If the contribution of another species is remarkable, then fully include the species in the profile retrieval.

If the second opportunity is applied (as in version 3.0), all entries with respect to main gases are completed with the information content about the additional main gases which had been taken into account.

3.2.3 Entry # 15, 16, and 17: Tangent height, pressure, and temperature

The retrieval in the current processor version (3.0) is performed on a layer grid which means that the profile results are assigned to atmospheric layers. Other retrieval schemes allow the assignment to atmospheric levels. All three quantities are provided for the layers which had been used for the retrieval. Tangent height and tangent pressure are given at the lower boundary of the layer. Since TOA is fixed at 100 km, an additional height level is provided. Pressure is derived from climatological information (see entry #8) which allows also the assignment of pressure at TOA. The temperature is given for each layer under the assumption of a homogeneous atmosphere for each layer.

3.2.4 Entry # 18: Main species for retrieval

This entry comprises the retrieval results with respect to the main species. Note that some limb applications make use from the opportunity to retrieve more than one main species. This has to be taken into account for the extraction of data from this data. The number of main species is given in entry #11.

3.2.5 Entry # 20: Measurement grid

This entry comprises the information about the grid on which the measurements are performed. Those can not been used for any conversion of retrieval results to another grid, since the results are provided on the retrieval grid.

3.2.6 Entry # 34: Additional Diagnostics

The entry "Additional diagnostics" shall allow the provision of additional helpful information. With version 3.0 some extensions to that dynamically defined entry had been introduced. The extension had been added at the end of the before defined content so that users who don't care of the extensions, can further use their own extraction tools.

As noted above in sub-section 2.2, there are eight sub-entries in this particular entry. The variable *ADDDIAG* is assigned in the following to that entry as an array of floats. *ADDDIAG* is written in following order:

1. *ADDDIAG(1)* – degree of freedom
2. *ADDDIAG(2)* – information content (is currently fixed to 1.0)
3. *entry = 2*
4. Diagonal of Averaging kernel (*AVK*)
   do k = 1,nstvec
   ADDDIAG(k+entry) = AVK(k,k)
   end do
   entry = entry + n_{stvec}
5. Number density for each main gas at each retrieval layer (*NRDENS*)
   k = 0
   do j = 1, n_1
   do i = ,n_{main}
   k = k+1
   ADDDIAG(entry+k) = NRDENS(j,i)
   end do

end do
*entry = entry + n1*n_{main}*

6. Initial number density for each main gas at each retrieval layer (*NRDENSINIT*)

k = 0
do j = 1,n_1
do i = 1, n_{main}
k = k+1
ADDDIAG(entry+k) = NRDENSINIT(j,i)
end do
end do
*entry = entry + n_1*n_{main}*

7. Conversion factors from partial columns to VMR at retrieval layers

do k = 1, n_{main}
ADDDIAG(entry+k) = s_k^{vmr}
end do
entry = entry + n_{main}

8. Conversion factors from partial columns to number density at retrieval layers

do k = 1, n_{main}
ADDDIAG(entry+k) = s_k^{nd}
end do
entry = entry + n_{main}

9. Averaging kernel of each main gas at each retrieval layer

k = 0
do j = 1,n_1
block = (j-1)n_{main}*
do i = 1,n_{main}
k = k +1
ADDDIAG(entry+k) = AVK(block+i,block+j)
end do
end do

4 Retrieval results and representation

All retrieval methods for the profile derivation from SCIAMACHY Limb measurements are non-linear. This means that their results must be interpreted and compared with respect to the selected approach. In the following, we have a collection of conversions between different representations. We like to emphasize that it is not an easy task to transform between retrievals performed on layers and retrievals derived on levels. For every transformation between different representation, care has to be taken which product entries are selected. It is absolutely mandatory that the measurement and retrieval grids are not mixed in any case: The measurement grid is provided to users' convenience to be informed about the height grid on which the measurement had been performed. The pressure and temperature is then derived by interpolation on the measurement grid entries.

4.1 Conversion between layer and level representation

One important issue for the correct interpretation of retrieval results is the conversion between different result representations. The conversion between partial column (or vertical column) and number density or volume mixing ratio at each retrieval layer had been shown; and conversion factors are provided. We note that the conversion is explicitly related to the transformation between the quantities assigned to retrieval layers. This does not show any direct transformation for quantities assigned to retrieval layers on one hand and for quantities related to retrieval levels on the other side.

It shall be noted that the profile retrieval is performed for height layers instead of height levels as in other context. Thus, the transformation must be found between those representations for comparability. In case of the SCIAMACHY Level 2 product, we propose to transform to the SCIAMACHY representation – if suitable -, since then any changes to the SCIAMACHY product can be avoided which can be caused by inter- or extrapolations to height levels. For that, one can start with the number density representation which is also provided in the product in the entry "Additional Diagnostics". In order to compare a SCIAMACHY profile in number density with a profile provided in number density per level, one can select between different opportunities from which we introduce two:

1. The profile which will be taken for the comparison with the SCIAMACHY product will be interpolated to the height grid of the SCIAMACHY retrieval grid (entry # 15). In a second step, the arithmetical mean for two neighboured levels is built to yield the profile result for the retrieval layers for comparison.
2. An interpolation (for example B-spline) of the profile which will be taken for the comparison with the SCIAMACHY product is applied over the total range of the height retrieval grid. The interpolation is then followed by the integration over each layer for the determination of the mean value per layer.

The second opportunity is a more accurate approach and is recommended to follow, if retrieval based on layers from that size is compared to profiles on a denser level grid.

4.2 Conversion of Averaging

Finally, short notice shall be given to the conversion of the provided averaging kernel. In sub-section 3.2.6, the content of the entry "Additional diagnostics" has been shown how it is constructed from the retrieval results. One part of the entry is the averaging kernel (AVK) provided in partial columns per layer. In order to re-calculate the averaging kernel for the

representation in number density (AVKNRDENS) and VMR (AVKVMR), two loops are given in the following:

Access to averaging kernel in "Additional Diagnostics":

```
k = 0
AVK(*,*) = 0.0
entry = 2*n_main*(n_1+1) + n_stvec + 2
do  j = 1,n_1
    block = (j-1)*n_main
    do i = 1,n_main
        k = k +1
        AVK(block+i,block+j) = ADDIAG(entry+k)
    end do
end do
```

Averaging kernel in number density (Access to first main gas result!):

```
entry =  2*n_main*n_1+ n_main + n_stvec + 2
do  k = 1, n_main
        s^nd(k) = ADDDIAG(entry+k)
end do
do  i = 1, n_main
        do  j = 1, n_main
                scale =s^nd(i) / s^nd(j)
                AVKNRDENS(i,j) = scale*AVK(i,j)
        end do
end do
```

Averaging kernel in volume mixing ratio (Access to first main gas result!):

```
entry =  2*n_main*n_1 + n_stvec + 2
do  k = 1, n_main
        s^vmr(k) = ADDDIAG(entry+k)
end do
do  i = 1, n_main
        do  j = 1, n_main
                scale =s^vmr(i) / s^vmr(j)
                AVKNRDENS(i,j) = scale*AVK(i,j)
        end do
end do
```