



PRODUCT USER MANUAL

Near real-time IASI total O₃ and O₃ profile HDF5

(O3M-44, O3M-306, O3M-49, O3M-315)

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1.1	10/02/2022	First version of the O ₃ PUM.
1.1	28/04/2022	CDOP-3 was removed from the document and IASI spatial resolution was corrected in Table 5, after RIDs from reviewers.
1.2	13/03/2025	New PUM for the HDF5 O ₃ products. Not reviewed.

RELATED PRODUCT LIST

Product ID	Product name	Instrument
O3M-44, O3M-306	IASI NRT total ozone	Metop B
O3M-49, O3M-315	IASI NRT ozone profile	Metop C

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1. INTRODUCTION

1.1 Purpose and scope

This document is the Product User Manual for the HDF5 Near Real Time IASI total O₃ and O₃ profiles retrieved within the context of the Satellite Application Facility on Atmospheric Composition Monitoring (AC SAF). This document gives a brief overview on the IASI retrieval algorithm and explains how to use and interpret the IASI O₃ profiles.

This document has been written as FORLI-O₃ 20191122_SP1 was running at EUMETSAT.

1.2 Acronyms

AC SAF: Atmospheric Composition Monitoring Satellite Application Facility

EUMETSAT: European Organisation for the Exploitation of Meteorological Satellites

EUMETCast: EUMETSAT multi-service data dissemination system

WMO: World Meteorological Organization

GTS: Global Telecommunication System

HDF5: Hierarchical Data Format

IASI: Infrared Atmospheric Sounding Interferometer

FORLI: Fast Optimal/Operational Retrievals on Layers for IASI

ULB: Université Libre de Bruxelles

LATMOS: Laboratoire Atmosphères, Milieux, Observations Spatiales

OEM : Optimal Estimation Method

DOFS : Degrees of Freedom for Signal

CP: Partial Column

TOA: Top Of the Atmosphere

VMR: Volume Mixing Ratio

1.3 Applicable and reference documents

1.3.1 Applicable documents

[AD1] FORLI Algorithm Theoretical Basis Document SAF/O3M/ULB/FORLI_ATBD Issue 1, 20/02/2014

[AD2] FORLI-O₃ Product Specification, Requirement And Assessment SAF/O3M/ULB/FORLIO3_PSRA Issue 1, 21/01/2015

[AD3] Product Requirements Document SAF/AC/FMI/RQ/PRD/001 Issue 1.6, 25/05/2022

[AD4] IASI total O₃ column validation report SAF/AC/AUTH/VR/001 Issue 1.

1.3.2 Reference documents

- [RD1] Hilton, F.; August, T.; Barnet, C.; Bouchard, A.; Camy-Peyret, C.; Clarisse, L.; Clerbaux, C.; Coheur, P.-F.; Collard, A.; Crevoisier, C.; Dufour, G.; Edwards, D.; Faijan, F.; Fourrié, N.; Gambacorta, A.; Gauguin, S.; Guidard, V.; Hurtmans, D.; Illingworth, S.; Jacquinet-Husson, N.; Kerzenmacher, T.; Klaes, D.; Lavanant, L.; Masiello, G.; Matricardi, M.; McNally, T.; Newman, S.; Pavelin, E.; Péquignot, E.; Phulpin, T.; Remedios, J.; Schlüssel, P.; Serio, C.; Strow, L.; Taylor, J.; Tobin, D.; Uspensky, A. & Zhou, D. Hyperspectral Earth Observation with IASI. *Bull. Am. Meteorol. Soc.*, 93(3), 347-370, doi: 10.1175/BAMS-D-11-00027.1, 2012.
- [RD2] Camy-Peyret, C. & Eyre, J. The IASI Science Plan. Technical report, A Report From The IASI Sounding Science Working Group, 1998.
- [RD3] Clerbaux, C.; Boynard, A.; Clarisse, L.; George, M.; Hadji-Lazaro, J.; Herbin, H.; Hurtmans, D.; Pommier, M.; Razavi, A.; Turquety, S.; Wespes, C. & Coheur, P. F. Monitoring of atmospheric composition using the thermal infrared IASI/MetOp sounder. *Atmos. Chem. Phys.*, 9(16):6041-6054, 2009.
- [RD4] Rodgers, C.D. Inverse methods for atmospheric sounding: Theory and Practice, Series on Atmospheric, Oceanic and Planetary Physics - Vol. 2. World Scientific, Singapore, New Jersey, London, Hong Kong, 2000.
- [RD5] Hurtmans, D.; Coheur, P.; Wespes, C.; Clarisse, L.; Scharf, O.; Clerbaux, C.; Hadji-Lazaro, J.; George, M. & Turquety, S. FORLI radiative transfer and retrieval code for IASI. *J. Quant. Spectrosc. Radiat. Transfer*, 113, 1391-1408, 2012.
- [RD6] Boynard, A., Hurtmans, D., Garane, K., Goutail, F., Hadji-Lazaro, J., Koukouli, M. E., Wespes, C., Vigouroux, C., Keppens, A., Pommereau, J.-P., Pazmino, A., Balis, D., Loyola, D., Valks, P., Sussmann, R., Smale, D., Coheur, P.-F., and Clerbaux, C.: Validation of the IASI FORLI/EUMETSAT ozone products using satellite (GOME-2), ground-based (Brewer–Dobson, SAOZ, FTIR) and ozonesonde measurements, *Atmos. Meas. Tech.*, 11, 5125–5152, <https://doi.org/10.5194/amt-11-5125-2018>, 2018.
- [RD7] EUMETCast Dissemination facility
<http://www.eumetsat.int/website/home/Data/DataDelivery/EUMETCast/index.html>

2. INTRODUCTION TO EUMETSAT SATELLITE APPLICATION FACILITY ON ATMOSPHERIC COMPOSITION MONITORING (AC SAF)

Background

The monitoring of atmospheric chemistry is essential due to several human caused changes in the atmosphere, like global warming, loss of stratospheric ozone, increasing UV radiation, and pollution. Furthermore, the monitoring is used to react to the threads caused by the natural hazards as well as follow the effects of the international protocols.

Therefore, monitoring the chemical composition and radiation of the atmosphere is a very important duty for EUMETSAT and the target is to provide information for policy makers, scientists and general public.

Objectives

The main objectives of the AC SAF is to process, archive, validate and disseminate atmospheric composition products (O_3 , NO_2 , SO_2 , BrO, HCHO, H_2O , OCIO, CO, NH_3), aerosol products and surface ultraviolet radiation products utilising the satellites of EUMETSAT. The majority of the AC SAF products are based on data from the GOME-2 and IASI instruments onboard Metop satellites.

Another important task besides the near real-time (NRT) and offline data dissemination is the provision of long-term, high-quality atmospheric composition products resulting from reprocessing activities.

Product categories, timeliness and dissemination

NRT products are available in less than three hours after measurement. These products are disseminated via EUMETCast, WMO GTS or internet.

- Near real-time trace gas columns (total and tropospheric O_3 and NO_2 , total SO_2 , total HCHO, CO) and ozone profiles
- Near real-time absorbing aerosol indexes from main science channels and polarization measurement detectors
- Near real-time UV indexes, clear-sky and cloud-corrected

Offline products are available within two weeks after measurement and disseminated via dedicated web services at EUMETSAT and AC SAF.

- Offline trace gas columns (total and tropospheric O_3 and NO_2 , total SO_2 , total BrO, total HCHO, total H_2O) and ozone profiles
- Offline absorbing aerosol indexes from main science channels and polarization measurement detectors
- Offline surface UV, daily doses and daily maximum values with several weighting functions

Data records are available after reprocessing activities from the EUMETSAT Data Centre and/or the AC SAF archives.

- Data records generated in reprocessing
- Lambertian-equivalent reflectivity
- Total OCIO

Users can access the AC SAF offline products and data records (free of charge) by registering at the AC SAF web site.

More information about the AC SAF project, products and services: <http://acsaf.org/>

AC SAF Helpdesk: helpdesk@acsaf.org

Twitter: https://twitter.com/Atmospheric_SAF

3. IASI-FORLI RETRIEVAL ALGORITHM

3.1 IASI instrument

IASI is an infrared Fourier transform spectrometer developed jointly by CNES (the French spatial agency) with support of the scientific community (for a review see [RD1]), and by EUMETSAT. IASI is mounted on-board the European polar-orbiting Metop satellite with the primary objective to improve numerical weather predictions, by measuring tropospheric temperature and humidity with high horizontal resolution and sampling, with 1 km vertical resolution, and with respectively 1 K and 10% accuracy [RD2]. IASI also contributes to atmospheric composition measurements for climate and chemistry applications [RD3]. To reach these two objectives, IASI measures the infrared radiation of the Earth's surface and of the atmosphere between 645 and 2760 cm^{-1} at nadir and along a 2200 km swath perpendicular to the satellite track. A total of 120 views are collected over the swath, divided as 30 arrays of 4 individual Field-of-views (FOVs) varying in size from $36 \times \pi\text{ km}^2$ at nadir (circular 12 km diameter pixel) to $10 \times 20 \times \pi\text{ km}^2$ at the larger viewing angle (ellipse-shaped FOV at the end of the swath). IASI offers in this standard observing mode global coverage twice daily, with overpass times at around 9:30 and 21:30 mean local solar time. The very good spatial and temporal sampling of IASI is complemented by fairly high spectral and radiometric performances: the calibrated level 1C radiances are at 0.5 cm^{-1} apodized spectral resolution (the instrument achieves a 2 cm optical path difference), with an apodized noise that ranges below 2500 cm^{-1} between 0.1 and 0.2 K for a reference blackbody at 280 K [RD1].

3.2 FORLI overview

FORLI (Fast Optimal/Operational Retrievals on Layers for IASI) is a radiative transfer model based on precalculated LUTs capable of processing in near-real-time the numerous radiance measurements made by the high-spatial and high-spectral resolution IASI, with the objective to provide global concentration distributions of atmospheric trace gases. For the inversion step, it relies on a scheme based on the widely used Optimal Estimation theory [RD4]. Three versions of the software have been set-up to process IASI level 1C radiances in near-real-time, for vertical profile retrievals of CO, O₃ and HNO₃.

The algorithm description with the methods used for forward and inverse modelling is given in the FORLI ATBD [AD1] and in [RD5].

4. IASI LEVEL 2 NRT O₃ PRODUCT

4.1 HDF5 PDU file name convention

The names of the IASI Level 2 O₃ products distributed on EUMETCast follow this example:

W_XX-EUMETSAT- Darmstadt,SOUNDING+SATELLITE,METOP*+IASI_C_EUM*letter*_
 yyyyymmddhhmmss_nnnnn_ACSAF_FORLI-O₃_12.h5

where:

<i>yyyyymmdd</i>	the UTC year, month, day of the data start sensing time
<i>hhmmss</i>	the UTC hour, minute, second of the data start sensing time
<i>nnnnn</i>	the orbit number
<i>*</i>	A, B or C
<i>letter</i>	C for commissioning, P for operational, R for secondary or redundant

4.2 HDF5 file size estimate

The size of the output may vary and is on average 1.3 G with a number of 480 files per day per instrument.

4.3 Description of the content of the HDF5 PDU file

In this table, the new HDF5 file variables are given with the equivalent BUFR variables. The FORLI-O₃ product descriptors are provided in the 11 last fields (in bold).

Molecule prefixes are removed in HDF5 files to reduce file size (One molecule - One file) e.g.:
 O₃_CP_O₃_A -> CP_mol_A.

Table 1: Data descriptors of IASI Level 2 O₃ BUFR file with equivalent HDF5 variables.

#	BUFR DATA DESCRIPTOR		NAME USED HEREAFTER in the PUM	Equivalent HDF5 field
0	0-0-1007	SATELLITE IDENTIFIER		
1	0-0-1031	IDENTIFICATION OF ORIGINATING/ GENERATING CENTRE		
2	0-25-060	SOFTWARE IDENTIFICATION		
3	0-0-2019	SATELLITE INSTRUMENTS		
4	0-0-2020	SATELLITE CLASSIFICATION		
5	0-0-4001	YEAR		/location/date

6	0-0-4002	MONTH		
7	0-0-4003	DAY		
8	0-0-4004	HOUR		/location/time
9	0-0-4005	MINUTE		
10	0-0-4006	SECOND		
11	0-0-5040	ORBIT NUMBER		/location/orbit
12	2-0-1133	#N/A		
13	0-0-5041	SCAN LINE NUMBER		/location/scanline
14	2-0-1000	#N/A		
15	0-0-5001	LATITUDE (HIGH ACCURACY)		/location/latitude
16	0-0-6001	LONGITUDE (HIGH ACCURACY)		/location/longitude
17	0-0-5043	FIELD OF VIEW NUMBER		1
18	0-0-7024	SATELLITE ZENITH ANGLE		/geometry/metop/zenith
19	0-0-5021	BEARING OR AZIMUTH (DEGREE TRUE)		/geometry/metop/azimuth
20	0-0-7025	SOLAR ZENITH ANGLE		/geometry/sun/zenith
21	0-0-5022	SOLAR AZIMUTH (DEGREE TRUE)		/geometry/sun/azimuth
22	0-0-7007	HEIGHT (Surface altitude in meter)		/location/surface altitude
23	0-4-0056	GENERAL RETRIEVAL QUALITY FLAG	O3_QFLAG	/fitted/diagnostics/QFLAG
24	0-4-0058	NUMBER OF VECTORS DESCRIBING THE CHAR. MATRICES	O3_NPCA	/fitted/characterisation/NPCA
25	0-4-0059	NUMBER OF LAYERS ACTUALLY RETRIEVED	O3_NFITLAYERS	/fitted/NFITLAYERS ²
26	0-4-0060	NUMBER OF O3 PROFILES RETRIEVED IN SCANLINE	O3_NBR	
27	0-4-0054	POTENTIAL PROCESSING AND INPUT ERRORS	O3_BDIV_LO	/fitted/diagnostics/BDIV
28	0-4-0055	DIAGNOSTICS ON THE RETRIEVAL	O3_BDIV_HI	
29	1-0-3019	#N/A REPEAT NEXT 3 19 TIMES		

30	0-4-0061	AIR PARTIAL COLUMNS ON EACH RETRIEVED LAYER	O3_CP_AIR	/fixed/CP_AIR ³
31	0-4-0062	A-PRIORI PARTIAL COLUMNS FOR O3 ON EACH RETRIEVED LAYER	O3_CP_O3_A	/fixed/CP_mol_A ³
32	0-4-0063	SCAL. VEC. MULT. A-PRI. O3 VEC. DEF. RETR. O3 VEC.	O3_X_O3	/fitted/X_mol
33	1-0-1010	#N/A REPEAT NEXT 1 10 TIMES		
34	0-4-0064	MAIN EIGENVALUES OF THE SENSITIVITY MATRIX	O3_H_EIGENVALUES	Fixed to 1
35	1-0-1190	#N/A REPEAT NEXT 1 190 TIMES		
36	0-4-0065	MAIN EIGENVECTORS OF THE SENSITIVITY MATRIX	O3_H_EIGENVECTORS	/fitted/characterisation/H_EIGENVECTORS
		Supplemental		
	N/A	Estimation of tropopause altitude (km)		/fixed/tropopause
	N/A	Pressure at each level defining layers (hPa)		/fixed/pressures

1 Structured data so no need

2 <0 if no fitted profile

3 Units are molecules/cm²

Usual FORLI-O₃ products have to be reconstructed/calculated from these above mentioned fields, see Section 5.

5. THE FORLI-O₃ PRODUCT

5.1 Product description

The product FORLI-O₃ includes several variables, described in Table 1 (bold) and in Table 2. The principal product is a vertical profile of O₃ provided on 41 layers, from the ground to 40 km with an additional layer from 40 km to TOA. In order to allow a rational use each retrieved profile is associated with averaging kernels and posterior error covariance matrices following the characterization of the optimal estimation. **For saving space, the matrices are compressed and have to be reconstructed using eigenvectors and eigenvalues of the sensitivity matrix (“MAIN EIGENVECTORS OF THE SENSITIVITY MATRIX” and “MAIN EIGENVALUES OF THE SENSITIVITY MATRIX”).** Each retrieval has also associated retrieval flags.

Note that the retrievals are performed on the basis of the *a priori* partial columns (“A-PRIORI PARTIAL COLUMNS FOR O₃ ON EACH RETRIEVED LAYER” called hereafter *CP_mol_A*), which are scaled individually using a *multiplication factor* (“SCAL. VEC. MULT. A-PRI. O₃ VEC. DEF. RETR. O₃ VEC” called hereafter *X_mol*). The multiplication factor equals therefore 1 at initial stage, is unitless, and should remain close to unity in normal circumstances. This ensures homogeneity of the retrieved values all along the altitudes, even when molecular amounts spans several decades. The content of *CP_mol_A* is computed using ray tracing methods described in the ATBD [AD1], while *X_mol* is retrieved using OEM method in a logarithmic space in order to avoid nonphysical negative values.

Table 2: Description and units of FORLI-O₃ product available in the IASI L2 O₃ HDF5 files

Name	Description	Units
QFLAG	General quality flag	N/A
BDIV	Potential processing and input errors and diagnostics on the retrieval	N/A
NPCA	Number of vectors describing the characterization matrices	N/A
NFITLAYERS	Number of layers actually retrieved; ≤ 19	N/A
CP_AIR	Air partial column on each retrieved layer	molecules /cm ²
CP_mol_A	A priori partial columns for O ₃ on each retrieved layer	molecules /cm ²
X_mol	Scaling vector multiplying the a priori O ₃ vector in order to define the retrieved O ₃ vector	N/A
H_EIGENVECTORS	Main eigenvectors of the sensitivity matrix	N/A
pressures	Pressure at each level defining layers	hPa
tropopause	Estimation of tropopause altitude	km

In Table 2 QFLAG is a single code assessing the quality of the retrieved profiles namely 2 for best quality pixels, 1 for valuable pixels and 0 for bad quality pixels. QFLAG is a FORLI-O₃ output, see Section 5.3.1.

Table 3: Potential processing and inputs errors in FORLI-O₃ (BDIV). Note that bits have been reassigned with new WMO descriptor bits.

Name	Value	Bit	WMO bit	Description	Comment
General					
AMP_ERROR	1	0	1	An error has been detected	
Origin					
AMP_L1	2	1	2	Message from L1	
AMP_L2	4	2	3	Message from L2	
AMP_ANC	8	3	4	Message from ancillary data	
AMP_FIT	16	4	5	Message from fitting procedure	
Input content					
AMP_QUALFLAG	256	8	7	Quality flag	Either bad L1 (qFlag) or L2 (F IASI Bad) flag raised
AMP_LINREG_L2	512	9	8	Level 2 “from linear regression” (F_Qual), report a pixel where L2 are not fully trusted	
AMP_EMPTY	1024	10	9	Empty field or data	Indicate missing T or humidity level(s) in the vertical profile
AMP_INCOMPLETE	2048	11	10	Missing surface pressure value	
AMP_RADFILTER	4096	12	11	Radiance filtering	Not used in this context
AMP_POLES	8192	13	12	Polar regions	Not used in this context
AMP_NIGHT	16384	14	13	Location in the night	Not used in this context
AMP_NEGZO	32768	15	14	Negative altitude	Surface below m.s.l.
AMP_COVERAGE	65536	16	15	Cloud covered scene	
AMP_SEA	131072	17	16	Scene above the sea	Not used so far
AMP_DESERT	262144	18	17	Scene above desert	
AMP_TSKIN	524288	19	18	Skin temperature	Missing skin temperature, start from BT
AMP_TDIFF	1048576	20	19	Skin temperature differential	Retrieved skin T too different from model
AMP_CONTRAST	2097152	21	20	Spectral line contrast too weak	No lines seen on spectrum (polar regions)
Fitting					
AMP_ITERATIONS	4194304	22	21	Maximum number of iterations exceeded	
AMP_NEGPC	8388608	23	22	Negative partial columns	
AMP_CONDITION	16777216	24	23	Matrix ill conditioned	
AMP_DIVERGED	33554432	25	24	Fit diverged	
AMP_GSL	67108864	26	25	Error in gsl usage	
AMP_BIAS	134217728	27	26	Residuals “biased”	
AMP_SLOPE	268435456	28	27	Residuals “sloped”	
AMP_RMS	536870912	29	28	Residuals rms large	
AMP_AVK	1073741824	30	29	Weird averaging kernels	
AMP_ICE	2147483648	31	30	Ice presence detected	

5.2 How to get the FORLI-O₃ products I need?

Table 4: FORLI-O₃ products that can be obtained from the HDF5 PDU files.

FORLI-O ₃ products	Notation	How to get/calculate it?	From
O ₃ profile (molecules/cm ²)	O3_CP_O3	see Section 5.2.1, Eq 1	OZO
O ₃ profile (VMR)	O3_VMR_O3	see Section 5.2.1, Eq 2	
O ₃ total column (molecules/cm ²)	O3_TC	see Section 5.2.1, Eq. 3	
A priori profile (molecules/cm ²)	CP_mol_A	Field "A-PRIORI PARTIAL COLUMNS FOR O3 ON EACH RETRIEVED LAYER"	
A priori profile (VMR)	O3_VMR_O3_A	See Section 5.2.3.2, Eq 10	
Averaging Kernel matrix in scaling factor	A	see Section 5.2.2, Eq.6	
Averaging Kernel matrix in partial column	A _{PC}	see Section 5.2.3.1, Eq. 9	
Averaging Kernel matrix in VMR	A _{VMR}	see Section 5.2.3.2, Eq. 12	
Total column averaging kernel vector	k	See Section 5.2.3.3, Eq. 13	
Degrees Of Freedom of the Signal	DOFS	trace(A) = trace(A _{PC}) = trace(A _{VMR})	
Absolute total retrieval error on the total column	σ _{TC}	See Section 5.2.3.3, Eq. 14	
Relative error profile (relative to the retrieved O3 profile in molecules/cm ² or VMR)	σ	See Section 5.2.2, Eq. 7	
Pressure levels	P	Field 'pressures', see Section 5.2.3.4	
Tropopause		Field 'tropopause'	

5.2.1 Reconstruction of the O₃ profile and calculation of the total column

The final **partial column profile** (molecules/cm²) is to be reconstructed by multiplying element-wise the two vectors defined earlier e.g.:

$$O3_CP_O3_i = CP_mol_A_i \times X_mol_i \quad \forall i \quad (1)$$

Profile spans *NFITLAYERS* layers, sampled on a 1 km grid, except the first one which starts from surface altitude and hence could be thinner, and the last one which extends up to TOA.

To convert this profile in VMR:

$$O3_VMR_O3_i = O3_CP_O3_i \div CP_AIR_i \quad \forall i \quad (2)$$

The **O₃ total column** (molecules/cm²) is obtained by summing the partial columns defined in Eq (1) on all retrieved layers:

$$O3_TC = \sum_i O3_CP_O3_i \quad (3)$$

5.2.2 Reconstruction of the characterisation matrices

Averaging kernel, which is normally an asymmetric matrix (*NFITLAYERS* × *NFITLAYERS*), is compressed by using a principal component decomposition representation. A reduced subset of principal vectors (*NPCA* out of *NFITLAYERS*) of the sensitivity matrix, *H*, is retained in order to achieve a meaningful compression. The averaging kernel matrix, *A*, is then reconstructed. The posterior variance-covariance matrix is also rebuilt during this procedure.

Reconstruction is done using the following formulation:

$$H = v \text{diag}(\lambda) v^T \quad (4)$$

$$\hat{S} = (H + S_a^{-1})^{-1} \quad (5)$$

$$A = \hat{S}H \quad (6)$$

where:

v is the principal eigenvectors matrix (*NFITLAYERS* × *NPCA*);

λ, the principal eigenvalues vector (*NPCA* × *NPCA*);

S_a, the *a priori* variance-covariance matrix;

Ŝ, the posterior variance-covariance matrix;

A, the averaging kernels matrix;

and *diag*(*x*) constructs a diagonal matrix the elements of which are given by the parameter vector *x*.

When the surface altitude > 1 km (i.e. *NFITLAYERS* < 41), users have to be careful and reduce *S_a* accordingly by decimating the first rows/columns corresponding to the unused altitude layers.

Eigenvectors matrix *v* is the *H_EIGENVECTORS* linear entry properly reshaped.

The *a priori* variance-covariance matrix *S_a* needed for the reconstruction is provided in Section 6.1.

Then the relative error profile can be calculated:

$$\sigma_i = \frac{\sqrt{\hat{s}_{i,i}}}{x_{mol_i}} \quad \forall i \quad (7)$$

As it is relative to the retrieval, the relative error profile is the same for the retrieved O₃ profile in molecules/cm² or VMR. It has therefore not to be recalculated.

A Python reading routine that reconstruct H, $\hat{S}$ and A is given in Section 6.2.

Reconstruction follows the same procedure as for CO using adapted vectors and matrices dimensions of 41 and 41x41 respectively. Due to the overwhelming size of such a document, they will not be given here. Users willing to have an example adapted for O₃ and/or HNO₃ can have them on request.

5.2.3 Unit conversions

All computations made in Section 5.2.2 were done in the unitless space of the multiplication factor. Users wishing to change the unit space should apply the following conversion rules:

5.2.3.1 Partial columns (molecules/cm²)

Partial column being defined by equation 1, it is easy to demonstrate that:

$$\hat{S}_{PC} = \text{diag}(CP_mol_A) \hat{S} \text{diag}(CP_mol_A) \quad (8)$$

$$A_{PC} = \text{diag}(CP_mol_A) A \text{diag}(CP_mol_A)^{-1} \quad (9)$$

5.2.3.2 Volume mixing ratios

Average volume mixing ratios (VMR) of the layers are computed as the ratios of the partial columns by the corresponding air partial columns. These latter are provided as CP_AIR . Hence conversions are given by:

$$O3_VMR_O3_A_i = CP_mol_A_i / CP_AIR_i \quad \forall i \quad (10)$$

$$\hat{S}_{VMR} = \text{diag}(O3_VMR_O3_A) \hat{S} \text{diag}(O3_VMR_O3_A) \quad (11)$$

$$A_{VMR} = \text{diag}(O3_VMR_O3_A) A \text{diag}(O3_VMR_O3_A)^{-1} \quad (12)$$

5.2.3.3 Total columns

The total column averaging kernel vector (k) is obtained by summing the rows of the averaging kernel matrix A :

$$k = (k_1 \ k_2 \ \dots \ k_{NFITLAYERS}),$$

with $k_i = A_{1,i} + A_{2,i} + \dots + A_{NFITLAYERS,i}$, $i=1$ to $NFITLAYERS$, (13)

The absolute total retrieval error (in molecules/cm²) on the total column is then calculated as σ_{TC}

$$\sigma_{TC} = \sqrt{\sum_{i,j} \hat{S}_{PC_{i,j}}} \quad (14)$$

5.2.3.4 Altitude-pressure conversion

The pressures per altitude are given in the Field ‘pressures’.

5.3 Using the product

5.3.1 Quality Flags for the retrieved profile

QFLAG is a single code assessing the quality of FORLI retrieved O₃ total column and profiles. QFLAG is a FORLI-O₃ output. It can be 2 (best quality), 1 (acceptable quality) or 0 (the rest).

QFLAG=2 for the most reliable pixels, in other words the best quality pixels. For the moment not used, in the future will be related to a cost function.

QFLAG=1 for the valuable pixels, to use with caution, *calculated as*:

- total cloud cover ≤13%
- flags AMP_ERROR+AMP_EMPTY+AMP_INCOMPLETE+AMP_NEGPC + AMP_CONDITION+ AMP_DIVERGED +AMP_AVK are null (see Tables 3a and 3b)
- RMS (residual rms) <3.5e-8
- DOFS>2
- -0.75e-9<BIAS (residual biased) <1.25e-9
- COL-06/COL TOT<0.085 (ratio of the partial column from ground to 6 km to the total column)

QFLAG=0 for the remaining pixels. We recommend not using these pixels.

For data validation or assimilation purposes, we recommend using the data with QFLAG equal to 2. For specific studies, if more pixels are needed, QFLAG equal to 1 can be used but analysis must consider the not optimal quality of these pixels.

5.4 Accuracy of the product

The requirements of the product are given in terms of threshold, target and optimal values in Table 5 below. This information is taken from the FORLI-O₃ product specification, requirement and assessment document [AD2] and is also given in the Product Requirements Document [AD3].

Table 5: FORLI-O₃ product requirements.

	Error* (%)			Spatial resolution	Spatial coverage	Cloud fraction	NRT
	Threshold	Target	Optimal				
Profile	30% stratosphere 50% troposphere	15% stratosphere 30% troposphere	5% stratosphere 10% troposphere	IASI spatial resolution	Global	< 13 %	< 3h
Total column	10%	5%	1%	IASI spatial resolution	Global	< 13 %	< 3h

*difference of quantity value obtained by measurement and true value of the quantity intended to be measured, as defined by CEOS/ISO:19159 (ISO/TS 19159-1:2014(en), Geographic information - Calibration and validation of remote sensing imagery sensors and data — Part 1: Optical sensors).

5.5 Validation of the product

The validation of the FORLI-O₃ product is performed jointly by AUTH (Aristotle University of Thessaloniki, Greece), DWD (Deutscher Wetterdienst, Germany) and RMI (Royal Meteorological Institute, Belgium). The IASI O₃ validation report [AD4] gives scientific validation results for IASI/Metop-A, IASI/Metop-B and IASI/Metop-C, total ozone products against the Dobson and Brewer spectrophotometer ground-based networks. In addition, comparison with the current GOME-2 O₃ product is provided. A more intensive validation exercise of total ozone and vertical profile products with satellite (GOME-2), ground-based (Dobson, Brewer, SAOZ, FTIR) and in situ data (ozonesonde) can be found in [RD6].

5.6 Product dissemination and archiving

5.6.1 Near real time Product dissemination

The IASI Level 2 products are disseminated to users in near real-time through EUMETCast [RD7] with a time lapse of two hours from sensing to delivery. The data is disseminated in HDF5 format. A full description of the IASI O₃ Level 2 HDF5 content is given in Section 4.3.

The dissemination of data will start in subsampled production (1 out of 10 pixels) due to existing computing capacity wrt timeliness requirements.

5.6.2 Archive retrieval

The IASI Level 2 products available from the EUMETSAT Data Centre are archived as full-dump products, but sub-setting capabilities are provided to the user in the retrieval process. The products in the EUMETSAT Data Centre are available to users for eight to nine hours after sensing.

6. APPENDICES

6.1 A priori variance-covariance matrix S_a used in the FORLI-O3 algorithm

```
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6.2 Reading routines in Python to reconstruct H, S and A

```
#!/usr/bin/env python3
```

```
r"""
```

```
Demo to read Forli H5 file
```

```
(c) GPC 2025-2037
```

```
\author Daniel R. Hurtmans <a href="linkURL">daniel.hurtmans@ulb.be</a>
```

```
\copyright {
```

```
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```

```
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    the compiled executable obtained from this code.
```

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liability, whether in an action of contract, tort or otherwise, arising from
out of or in connection with the software or the use or other dealings in
the software.

```
}  
"""
```

```
from contextlib import suppress  
from functools import partial  
from dataclasses import dataclass
```

```
import h5py  
import numpy as np
```

```
class Covar:  
    Sa = None
```

```
    def __len__(self) -> int:  
        return len(self.Sa)
```

```
class CovarO3(Covar):
```

```
    Sa = np.array(  
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+1.10840927e-02]]
)

```
def rebuild_derived_values(sa_inv: dict[int, np.ndarray], data: dict) -> None:
```

```
# Total Column
```

```
with suppress(KeyError):
```

```
    data['column'] = np.nansum(data['partial prior'] * data['raw x'], axis=1)
```

```
    data['column'][np.where(data['nfit_layers'] <= 0)[0]] = np.nan
```

```
    data['column'] = data['column'].reshape((-1, 1))
```

```
# Sensitivity and Relative AVK
```

```
with suppress(KeyError):
```

```
    size, nmaxfitlayers = data['partial prior'].shape
```

```
    data['rel kernels'] = np.full((size, nmaxfitlayers, nmaxfitlayers),  
                                  np.nan, dtype=np.double)
```

```
    data['sensitivity'] = np.full((size, nmaxfitlayers, nmaxfitlayers), np.nan,  
                                  dtype=np.double)
```

```
for i, eigen_vectors in enumerate(data['eigen vectors']):
```

```
    size = max(int(data['npca'][i][0]), 0) * int(data['nfit_layers'][i][0])
```

```
    if size > 0:
```

```
        sensitivity = eigen_vectors[0:size].reshape((data['npca'][i][0], -1))
```

```
        sensitivity = np.dot(sensitivity.T, sensitivity)
```

```
        start_pos = nmaxfitlayers - sensitivity.shape[0]
```

```
        s = slice(start_pos, None)
```

```
        data['rel kernels'][i, s, s] = (
```

```
            np.linalg.solve(sensitivity + sa_inv[start_pos], sensitivity))
```

```
        data['sensitivity'][i, s, s] = sensitivity
```

```
# Degrees of freedom of the signal
```

```
with suppress(KeyError):
    data['dofs'] = np.array([np.nansum(np.diag(i))
                            for i in data['rel kernels']]).reshape((-1, 1))
    data['dofs'][np.where(data['nfit_layers'] <= 0)] = np.nan

# Partial columns
with suppress(KeyError):
    data['partial'] = data['partial prior'] * data['raw x']

def read_hdf_file(file_path: str, imports: dict, process_extra) -> dict:
    def _read_hdf5_field(h5file: h5py.File, field_name: str) -> np.ndarray:
        field = h5file[field_name][()]
        # Reshape accordingly
        if len(field.shape) < 3:
            field = field.reshape((-1, 1))
        elif len(field.shape) == 3:
            field = field.reshape((-1, field.shape[2]))
        return field

    if len(imports) > 1:
        imports = {your_key: imports[your_key] for your_key in imports}

    data = {}
    with h5py.File(file_path, 'r') as h5file:
        for key, h5field in imports.items():
            data[key] = _read_hdf5_field(h5file, h5field)
    if process_extra:
        process_extra(data)
    return data

def read_forli_hdf(filename: str, covar: Covar):
    imports = {
        'date': '/location/date',
        'hhmmss': '/location/time',
        'orbit': '/location/orbit',
        'scanline': '/location/scanline',
        'latitude': '/location/latitude',
        'longitude': '/location/longitude',
        'zenithal': '/geometry/metop/zenith',
        'azimuth': '/geometry/metop/azimuth',
        'sun': '/geometry/sun/zenith',
        'sun_az': '/geometry/sun/azimuth',
        'gqf': '/fitted/diagnostics/QFLAG',
        'bdiv': '/fitted/diagnostics/BDIV',
        'z0': '/location/surface altitude',
        'npca': '/fitted/characterisation/NPCA',
        'nfit_layers': '/fitted/NFITLAYERS',
        'partial air': '/fixed/CP_AIR',
        'partial prior': '/fixed/CP_mol_A',
        'raw x': '/fitted/X_mol',
        'eigen vectors': '/fitted/characterisation/H_EIGENVECTORS',
        'tropo': '/fixed/tropopause',
        'pressures': '/fixed/pressures',
    }

    max_fit_layers = len(covar)
```

```
# Build inverses of covariance up to 8 km
sa_inv = {i: np.linalg.inv(covar.Sa[i - max_fit_layers:, i - max_fit_layers:])
          for i in range(9)}
return read_hdf_file(filename, imports, partial(rebuild_derived_values,
                                                sa_inv))

if __name__ == '__main__':
    filename = 'Forli_O3,METOPB+IASI_C_EUMP_20230808123555_56499_eps_o.h5'
    results = read_forli_hdf(filename, CovarO3())
    print(results['dofs'])
    print(results['rel kernels'])
```