ATMOSPHERIC COMPOSITION MONITORING

PRODUCT USER MANUAL

Near real-time IASI total O_3 and O_3 profile

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

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DOCUMENT STATUS SHEET

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1.0	04/06/2020	Draft version of the O_3 PUM.
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.

RELATED PRODUCT LIST

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

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1. INTRODUCTION

1.1 Purpose and scope

This document is the Product User Manual for the Near Real Time IASI total O_3 and O_3 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 O_3 profiles.

This document has been written as FORLI-O_3 v20151001_sp20171122 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
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-O_3 Product Specification, Requirement And Assessment SAF/O3M/ULB/FORLICO_PSRA Issue 1, 21/01/2015

[AD3] Product Requirements Document SAF/AC/FMI/RQ/PRD/001 Issue 1.6, 25/05/202

[AD4] IASI total O_3 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, OClO, CO, NH3), 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 OClO

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 $\times\pi$ km^2 at nadir (circular 12 km diameter pixel) to 10 x 20 x π 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, O_3 and HNO_3.

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 BUFR PDU file name convention

The names of the IASI Level 2 O_3 products distributed on EUMETCast follow this example:

W_XX-EUMETSAT- Darmstadt,SOUNDING+SATELLITE,METOP*+IASI_C_EUM*letter*_ *yyyymmdd*hhmmss_nnnnn_eps_o_ozo_l2.bin

where:

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

4.2 BUFR file size estimate

The size of the output may vary and is on average 2 Mb with a number of 480 files per day per instrument.

4.3 Description of the content of the BUFR PDU file

The IASI Level 2 O_3 BUFR PDU file structure is summarised below. The FORLI-O_3 product is provided in the last 11 fields (in bold).

Table 1: Data descriptors of IASI Level 2 O_3 BUFR file

#	DATA DESCRIPTOR		NAME USED HEREAFTER
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	
6	0-0-4002	MONTH	
7	0-0-4003	DAY	
8	0-0-4004	HOUR	
9	0-0-4005	MINUTE	
10	0-0-4006	SECOND	
11	0-0-5040	ORBIT NUMBER	

12	2-0-1133	#N/A	
13	0-0-5041	SCAN LINE NUMBER	
14	2-0-1000	#N/A	
15	0-0-5001	LATITUDE (HIGH ACCURACY)	
16	0-0-6001	LONGITUDE (HIGH ACCURACY)	
17	0-0-5043	FIELD OF VIEW NUMBER	
18	0-0-7024	SATELLITE ZENITH ANGLE	
19	0-0-5021	BEARING OR AZIMUTH (DEGREE TRUE)	
20	0-0-7025	SOLAR ZENITH ANGLE	
21	0-0-5022	SOLAR AZIMUTH (DEGREE TRUE)	
22	0-0-7007	HEIGHT (Surface altitude in meter)	
23	0-0-8046	ATMOSPHERIC CHEMICAL OR PHYSICAL CONSTITUENT TYPE	
24	**0-4-0056**	**GENERAL RETRIEVAL QUALITY FLAG**	**O3_QFLAG**
25	**0-4-0058**	**NUMBER OF VECTORS DESCRIBING THE CHAR. MATRICES**	**O3_NPCA**
26	**0-4-0059**	**NUMBER OF LAYERS ACTUALLY RETRIEVED**	**O3_NFITLAYERS**
27	**0-4-0060**	**NUMBER OF O3 PROFILES RETRIEVED IN SCANLINE**	**O3_NBR**
28	**0-4-0054**	**POTENTIAL PROCESSING AND INPUTS ERRORS**	**O3_BDIV_LO**
29	**0-4-0055**	**DIAGNOSTICS ON THE RETRIEVAL**	**O3_BDIV_HI**
30	**1-0-3041**	#N/A REPEAT NEXT 3 41 TIMES	
31	**0-4-0061**	**AIR PARTIAL COLUMNS ON EACH RETRIEVED LAYER**	**O3_CP_AIR**
32	**0-4-0062**	**A-PRIORI PARTIAL COLUMNS FOR O3 ON EACH RETRIEVED LAYER**	**O3_CP_O3_A**
33	**0-4-0063**	**SCAL. VEC. MULT. A-PRI. O3 VEC. DEF. RETR. O3 VEC.**	**O3_X_O3**
34	**1-0-1021**	#N/A REPEAT NEXT 1 21 TIMES	
35	**0-4-0064**	**MAIN EIGENVALUES OF THE SENSITIVITY MATRIX**	**O3_H_EIGENVALUES**
36	**1-0-2215**	#N/A REPEAT NEXT 2 215 TIMES	
37	**1-0-1004**	#N/A REPEAT NEXT 1 4 TIMES	
38	**0-4-0065**	**MAIN EIGENVECTORS OF THE SENSITIVITY MATRIX**	**O3_H_EIGENVECTORS**
39	**0-4-0065**	**MAIN EIGENVECTORS OF THE SENSITIVITY MATRIX**	**O3_H_EIGENVECTORS**

Usual FORLI-O_3 products have to be reconstructed/calculated from these above mentioned fields, see Section 5.

Among the other IASI Level 2 available products, temperature, humidity and cloud information needed to completely characterize FORLI-O_3 products can be found in files distributed by EUMETCast called:
W_XX-EUMETSAT- Darmstadt,SOUNDING+SATELLITE,METOP*+IASI_C_EUM*letter*_ *yyyymmdd*hhmmss_nnnnn_eps_o_<prod>_l2.bin

where:

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

product code <prod>	
twt	atmospheric temperature and water vapour
clp	cloud parameters

5. THE FORLI-O_3 PRODUCT

5.1 Product description

The product FORLI-O_3 includes several variables, described in Table 1 (bold) and in Table 2. The principal product is a vertical profile of O_3 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 *O3_CP_O3_A)*, which are scaled individually using a *multiplication factor* ("SCAL. VEC. MULT. A-PRI. O3 VEC. DEF. RETR. O3 VEC" called hereafter *O3*_X_*O3*). 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 span several decades. The content of *O3_CP_O3_A* is computed using ray tracing methods described in the ATBD [AD1], while *O3*_X_*O3* is retrieved using OEM method in a logarithmic space in order to avoid nonphysical negative values.

Table 2: Description and units of FORLI-O_3 product available in the IASI L2 O_3 BUFR files

Name	**Description**	**Units**
O3_QFLAG	General quality flag	N/A
O3_BDIV_LO	Potential processing and input errors	N/A
O3_BDIV_HI	Diagnostics on the retrieval	N/A
O3_NPCA	Number of vectors describing the characterization matrices	N/A
O3_NFITLAYERS	Number of layers actually retrieved; ≤ 41	N/A
O3_NBR	Number of O_3 profiles retrieved in scanline	N/A
O3_CP_AIR	Air partial column on each retrieved layer	moles /cm2
O3_CP_O3_A	A priori partial columns for O_3 on each retrieved layer	moles /cm2
O3_X_O3	Scaling vector multiplying the a priori O_3 vector in order to define the retrieved O_3 vector	N/A
O3_H_EIGENVALUES	Main eigenvalues of the sensitivity matrix	N/A
O3_H_EIGENVECTORS	Main eigenvectors of the sensitivity matrix	N/A

In Table 2 O3_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. O3_QFLAG is a FORLI-O_3 output, see Section 5.3.1.

Table 3a: Potential processing and inputs errors in FORLI-O_3 (O3_BDIV_LO). Note that bits have been reassigned with new WMO descriptor bits.

Name	Value	old 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	

Table 3b: Diagnostics on the retrieval of FORLI-O_3 (O3_BDIV_HI). Note that bits have been reassigned with new WMO descriptor bits.

Name	Value	old Bit	WMO bit	Description	Comment
Filtering					
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-O_3 products I need?

Table 4: FORLI-O_3 products that can be obtained from the BUFR PDU files.

FORLI-O3 products	Notation	How to get/calculate it?	From
O3 profile (moles/cm^2)	O3_CP_O3	see Section 5.2.1, Eq 1	ozo
O3 profile (VMR)	O3_VMR_O3	see Section 5.2.1, Eq 2	
O3 total column (moles/cm^2)	O3_TC	see Section 5.2.1, Eq. 3	
A priori profile (moles/cm^2)	O3_CP_O3_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 moles/cm^2 or VMR)	σ	See Section 5.2.2, Eq. 7	
Pressure levels	p	See Section 5.2.3.4, Eq. 16 to 18	twt

5.2.1 Reconstruction of the O_3 profile and calculation of the total column

The final **partial column profile** (moles/cm^2) is to be reconstructed by multiplying element-wise the two vectors defined earlier e.g.:

$$O3\_CP\_O3_i = O3\_CP\_O3\_A_i \times O3\_X\_O3_i \quad \forall i \tag{1}$$

Profile spans *O3_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:

$$O3\_VMR\_O3_i = O3\_CP\_O3_i \div O3\_CP\_AIR_i \quad \forall i \tag{2}$$

The **O_3 total column** (moles/cm^2) is obtained by summing the partial columns defined in Eq (1) on all retrieved layers:

$$O3\_TC = \sum_i O3\_CP\_O3_i \tag{3}$$

The total (or partial columns) can be similarly expressed in molecules/cm^2, in Dobson unit (DU) or in kg/m^2 by multiplying the values in moles/cm^2 by 6.02214086x10^{+23}, by 2.238714074x10^{+7} or by 280.1012135 respectively.

5.2.2 Reconstruction of the characterisation matrices

Averaging kernel, which is normally an asymmetric matrix (*O3_NFITLAYERS* × *O3_NFITLAYERS*), is compressed by using a principal component decomposition representation. A reduced subset of principal vectors (*O3_NPCA* out of *O3_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:

$$H = \nu \, \mathrm{diag}(\lambda) \, \nu^T \tag{4}$$
$$\hat{S} = (H + S_a^{-1})^{-1} \tag{5}$$
$$A = \hat{S}H \tag{6}$$

where:
- ν is the principal eigenvectors matrix (*O3_NFITLAYERS* × *O3_NPCA*);
- λ, the principal eigenvalues vector (*O3_NPCA* × *O3_NPCA*);
- S_a, the *a priori* variance-covariance matrix;
- $\hat{S}$, 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. O3_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 ν is the *O3_H_EIGENVECTORS* linear entry properly reshaped, and eigenvalues vector λ is the *O3_H_EIGENVALUES* entry.

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:

$$\sigma_i = \frac{\sqrt{\hat{S}_{i,i}}}{O3\_X\_O3_i} \quad \forall i \tag{7}$$

As it is relative to the retrieval, the relative error profile is the same for the retrieved O_3 profile in moles/cm^2 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 O_3 and/or HNO_3 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 (moles/cm^2)

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

$$\hat{S}_{PC} = diag(O3\_CP\_O3\_A)\,\hat{S}\;\,diag(O3\_CP\_O3\_A) \tag{8}$$
$$A_{PC} = diag(O3\_CP\_O3\_A)\;A\;diag(O3\_CP\_O3\_A)^{-1} \tag{9}$$

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 *O3_CP_AIR*. Hence conversions are given by:

$$O3\_VMR\_O3\_A_i = O3\_CP\_O3\_A_i / O3\_CP\_AIR_i \quad \forall i \tag{10}$$
$$\hat{S}_{VMR} = diag(O3\_VMR\_O3\_A)\,\hat{S}\;\,diag(O3\_VMR\_O3\_A) \tag{11}$$
$$A_{VMR} = diag(O3\_VMR\_O3\_A)A\;diag(O3\_VMR\_O3\_A)^{-1} \tag{12}$$

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*:

$$k = \left(k_1\;\;k_2\;\;\ldots\;\;k_{O_3\_NFITLAYERS}\right),$$
with $k_i = A_{1,i} + A_{2,i} + \ldots + A_{O3\_NFITLAYERS,i}$, i=1 to O3_NFITLAYERS, (13)

The absolute total retrieval error (in moles/cm^2) 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

Temperature and humidity vertical profiles extracted from **IASI L2 twt produc**t are given on 101 pressure levels (in Pa). To calculate the pressure levels corresponding to the altitude levels of the FORLI-O_3 retrievals, one should first calculate the altitude levels corresponding to the IASI L2 twt product.

From temperature and humidity vertical profiles (extracted from IASI L2 twt product), the correspondence between altitude and pressure could be calculated by iterating from the surface to the top of the atmosphere. The assumptions on the surface characteristics are:

surface altitude = z_0 ("HEIGHT", from BUFR files)
surface pressure = p_0 ("PRESSURE (HIGH PRECISION)" from IASI L2 twt product)
surface temperature = T_o, first level of the temperature profile T (extracted from IASI L2 twt product)
surface humidity = q_o, first level of the humidity profile q (extracted from IASI L2 twt product)

The acceleration due to the gravity is function of the geographic latitude ϕ and of the altitude z_i:

$$g(z_i, \phi) = g_\phi - (3.085462 \times 10^{-6} + 2.27 \times 10^{-9} \cos(2\phi))z_i$$
$$+(7.254 \times 10^{-13} + 1.0 \times 10^{-20} \cos(2\phi))\, z_i{}^2 - (1.517 \times 10^{-19} + 6 \times 10^{-22} \cos(2\phi))z_i{}^3 \quad (15)$$

where

$$g_\phi = 9.806160(1 - 0.0026373 \cos(2\phi) + 0.0000059 \cos^2(2\phi)) \text{ ms}^{-2} \quad (16)$$

The mean virtual temperature between two pressure levels p_i and p_{i+1} (just above level i) is then:

$$\overline{Tv_{\iota,\iota+1}} = \frac{T_i(1+0.608\, q_i)+T_{i+1}(1+0.608\, q_{i+1})}{2} \quad (17)$$

with T_i and q_i, the temperature and humidity at p_i, respectively, and T_{i+1} and q_{i+1}, the temperature and humidity at p_{i+1}, respectively.

Then the altitude of the pressure level p_{i+1} can be estimated from the pressure level p_i (just below level i+1):

$$z_{i+1} = z_i + \frac{R \times \overline{Tv_{\iota,\iota+1}}}{g(z_i,\phi)} \times \ln \frac{p_i}{p_{i+1}} \quad (18)$$

with R = 287.06 JK^{-1}kg^{-1}, the gas constant for dry air

We obtain the altitude profile corresponding to the IASI L2 twt product.
Then we can extract the pressure levels associated to IASI FORLI-O_3 product from the pressure vertical profile by using a cubic spline interpolation.

The conversion between pressure and height is done as in the “IASI Level2 Product Generation specification” document.

5.3 Using the product

5.3.1 Quality Flags for the retrieved profile

O3_QFLAG is a single code assessing the quality of FORLI retrieved O_3 total column and profiles. O3_QFLAG is a FORLI-O_3 output. It can be 2 (best quality), 1 (acceptable quality) or 0 (the rest).

O3_QFLAG=2 for the most reliable pixels, in other words the best quality pixels. For the moment <u>not used</u>, in the future will be related to a cost function.

O3_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)

O3_QFLAG=0 for the remaining pixels. We recommend not using these pixels.

For data validation or assimilation purposes, we recommend using the data with O3_QFLAG equal to 2. For specific studies, if more pixels are needed, O3_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-O_3 product specification, requirement and assessment document [AD2] and is also given in the Product Requirements Document [AD3].

Table 5: FORLI-O_3 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-O_3 product is performed jointly by AUTH (Aristotle University of Thessaloniki, Greece), DWD (Deutscher Wetterdienst, Germany) and RMI (Royal Meteorological Institute, Belgium). The IASI O_3 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 O_3 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 WMO (BUFR) format. A full description of the IASI O_3 Level 2 BUFR 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. Plans are to go full production during 2022.

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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-1.55041830e-03 -6.89173660e-04 7.05130740e-03 1.10803550e-02 1.24874820e-02 1.15020730e-02
8.87087600e-03 1.11864690e-03 -1.72809990e-02 -4.67017940e-02 -6.48370350e-02 -7.06370380e-02 -
7.48487060e-02 -8.17857940e-02 -8.82558410e-02 -9.24021210e-02 -9.09060160e-02 -8.23066640e-02 -
6.82574230e-02 -5.08571880e-02 -3.52636350e-02 -2.16525860e-02 -8.93427200e-03 2.30860050e-03
1.22743280e-02 2.13508020e-02 2.90665430e-02 3.53963980e-02 4.03082210e-02 4.35746710e-02
4.55704910e-02 4.63578100e-02 4.59736110e-02 4.42795260e-02 4.18641180e-02 3.90101810e-02
3.60622320e-02 3.26104890e-02 2.95601890e-02 2.61727970e-02 7.08700565e-03;
-1.10416420e-03 -3.38528910e-05 6.91493550e-03 1.00762980e-02 1.09206240e-02 9.66638330e-03
7.25725550e-03 5.60643830e-04 -1.52587280e-02 -4.05531580e-02 -5.55341740e-02 -5.95539630e-02 -
6.25845430e-02 -6.82387580e-02 -7.36124940e-02 -7.70454290e-02 -7.56910460e-02 -6.83109820e-02 -
5.63680070e-02 -4.15764860e-02 -2.83239190e-02 -1.67489360e-02 -5.93385850e-03 3.58258320e-03
1.18969330e-02 1.93503580e-02 2.55672120e-02 3.05331150e-02 3.42810450e-02 3.67106700e-02
3.81570170e-02 3.86914310e-02 3.83454520e-02 3.70140980e-02 3.51532600e-02 3.30019300e-02
3.08312720e-02 2.82883620e-02 2.61727970e-02 2.38052950e-02 7.94361408e-03;
3.71254550e-03 3.41629837e-03 5.17981497e-03 5.01996838e-03 4.01331378e-03 2.09588537e-03
4.68012767e-04 -2.76679346e-03 -1.07124776e-02 -2.29238276e-02 -2.70210087e-02 -2.21019300e-02 -
1.67392046e-02 -1.30619144e-02 -1.07139874e-02 -9.12976283e-03 -7.89632209e-03 -6.76772549e-03 -
5.14296457e-03 -2.85893296e-03 -4.45332526e-04 1.82265152e-03 4.09821215e-03 6.00248266e-03
7.41624628e-03 8.31022897e-03 8.79772472e-03 8.82674905e-03 8.36643346e-03 7.76113317e-03
7.19308378e-03 6.70979102e-03 6.25738742e-03 6.02865638e-03 5.86766152e-03 5.83916581e-03
6.09296394e-03 6.37213622e-03 7.08700565e-03 7.94361408e-03 1.10840927e-02];

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

```
#!/usr/bin/python
#-*- coding:utf-8 -*-

## This script read the compressed H matrix (eigenvalues and eigenvectors) for two cases from the file 'OZO.inp'
## normally these will be read from the Forli O3 products (O3_H_EIGENVALUES and O3_H_EIGENVECTORS)

## It then reconstructs H and show how to compute the retrieval error covariance matrix, S, and the
## averaging kernel, A

import sys
from numpy import *
from numpy.linalg import *

from Sa_O3 import * ## Get the apriori error covariance matrix Sa

line_type=0
with open('OZO.inp','r') as f:
    for line in f:
        if line[0]=='#':
            comment=line.replace("\n", " ")
            continue
        if line_type==0:
            E=fromstring(line,dtype=float, sep=',') ## E (O3_H_EIGENVALUES)
            line_type=1
        elif line_type==1:
            V=fromstring(line,dtype=float, sep=',') ## V (O3_H_EIGENVECTORS)
            line_type=2
        if line_type==2:
            line_type=0

            nEvals=sum(isfinite(E))  # number of eigenvalues/eigenvectors (of H)
            nEvecs=sum(isfinite(V))  # total number of elements in the eigenvectors (of H)
            nAlts=nEvecs/nEvals      # length of each eigenvector (i.e. number of altitudes)
            nSkip=int(41-nAlts)

            E=E[:nEvals]
            V=V[:nEvecs].reshape((nEvals,nAlts))

            ## H = V'EV (reconstruct H from eigendecomposition)
            H=dot(dot(V.T,diag(E)),V)

            Sa_Local=Sa[nSkip:,nSkip:] # skip altitudes below surface from Sa, the apriori error covariance matrix

            ## S = (H + Sa^-1)^-1   (retrieval error covariance matrix)
            S=inv(H+inv(Sa_Local))

            ## A = SH  (averaging kernel)
            A=dot(S,H)

            print(comment)
            print("S = ",S)
            print("A = ",A)
            print("DOFS = ",trace(A))
```