PRODUCT USER MANUAL
IASI reprocessed L2 O_3 CDR
(O3M-520.1, O3M-521.1) Metop-A&B

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DOCUMENT STATUS SHEET

Issue	Date	Modified items / Reason for change
1.0	19/03/2025	First version of the IASI O3 Level 2 CDR PUM
1.1	04/04/2025	Version submitted for review to EUMETSAT

RELATED PRODUCT LIST

Product ID	Product name
O3M-44	IASI NRT total O3 Metop-A&B
O3M-49	IASI NRT O3 profile Metop-A&B

Introduction to EUMETSAT Satellite Application Facility on Atmospheric Composition monitoring (AC SAF)

The Atmospheric Composition Satellite Application Facility (AC SAF), a part of EUMETSAT, is dedicated to monitoring and analysing key atmospheric components such as ozone, trace gases, aerosols, and ultraviolet radiation. These observations contribute to understanding climate change, air quality, and the health of the environment on both regional and global scale.

Background

Monitoring atmospheric composition has become critical in understanding and mitigating the impacts of both anthropogenic and natural changes to the Earth's atmosphere. Human activities, such as combustion of fossil fuels and industrial pollution, contribute to global warming, the depletion of stratospheric ozone, and an increase in harmful ultraviolet (UV) radiation. In addition, natural hazards like volcanic eruptions and forest fires release pollutants that can affect air quality and climate on regional and global scales.
Accurate and continuous monitoring of atmospheric chemistry and radiation is essential for tracking these changes and assessing the effectiveness of international environmental agreements such as the Montreal Protocol and the Paris Agreement. AC SAF plays a crucial role in this process by providing reliable, timely data to policymakers, scientists, and the general public. These data are indispensable for informed decision-making on environmental protection, climate mitigation strategies, and public health initiatives.

Objectives

The primary objectives of the AC SAF are to process, archive, validate, and disseminate high-quality atmospheric data, including gaseous compounds, aerosols and surface radiation. These products, derived from EUMETSAT satellites such as Metop and future platforms (MTG, EPS-SG), are critical for environmental research, public health, and policy decisions.

The objective is reached by providing near real-time (NRT) data as well as long-term, high-quality atmospheric composition data records.

Product categories, timeliness

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

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

Data records are available from the AC SAF archives after reprocessing or dedicated data record generation activities.

Data availability

All AC SAF data is freely available to users worldwide. To access the data, interested users need to register through the AC SAF website. More detailed information on data access, product specifications, and registration can be found at http://ac-saf.eumetsat.int/ by selecting 'Data access'.

AC SAF WWW site: http://ac-saf.eumetsat.int/
AC SAF on X: @Atmospheric_SAF
AC SAF Helpdesk: helpdesk@acsaf.org

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1. INTRODUCTION

1.1 Purpose and scope

This document is the Product User Manual for reprocessed IASI Level 2 ozone climate data record (L2 O_3 CDR) produced within the context of the Satellite Application Facility on Atmospheric Composition Monitoring (AC SAF) fourth Continuous Development and Operations Phase (CDOP-4). This document gives a brief overview on the IASI O_3 retrieval algorithm and explains how to use and interpret the reprocessed IASI O_3 CDR.

The IASI O_3 CDR (DOI: 10.15770/EUM_SAF_AC_0051) is produced at EUMETSAT using the Metop-A&B NRT IASI FORLI-O_3 v20151001.

The reprocessing for Metop-A and Metop-B covers the following dates:

	IASI-A	IASI-B
Start date	10/07/2007	20/02/2013
End date	31/12/2019	31/12/2023

1.2 Acronyms

AC SAF	Atmospheric Composition Monitoring Satellite Application Facility
BIRA	Belgian Institute for Space Aeronomy
CDOP-4	fourth Continuous Development and Operations Phase
CDR	Climate data record
CNES	Centre National d’Études Spatiales
CP	Partial Column
DOFS	Degrees of Freedom for Signal
FORLI	Fast Optimal Retrievals on Layers for IASI
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
GTS	Global Telecommunication System
IASI	Infrared Atmospheric Sounding Interferometer
LATMOS	Laboratoire Atmosphères, Observations Spatiales
NetCDF	Network Common Data Form
NRT	Near Real Time
OEM	Optimal Estimation Method
TOA	Top Of the Atmosphere
ULB	Université Libre de Bruxelles
VMR	Volume Mixing Ratio
WMO	World Meteorological Office

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] IASI O_3 NRT PUM SAF/AC/ULB/PUM/003 Issue 1.1, 28/04/2022

[AD3] Product Requirements Document SAF/AC/FMI/RQ/PRD/001 Issue 1.9.1, 03/02/2022

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] EUMETSAT Data Store https://www.eumetsat.int/eumetsat-data-store

[RD7] 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. & Clerbaux, C. Validationof 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, 2018.

[RD8] Boynard, A.; Wespes, C.; Hadji-Lazaro, J.: Sinnathamby, S.; Hurtmans, D.; Coheur, P.-F.; Doutriaux-Boucher, M.; Onderwaater, J.; Steinbrecht, W.; Pennington, E. A.; Bowman, K. & Clerbaux, C. Tropospheric Ozone Assessment Report (TOAR): 16-year ozone trends from the IASI Climate Data Record. *EGUsphere [preprint]*, https://doi.org/10.5194/egusphere-2025-1054, 2025.

2. IASI Reprocessed O_3 CDR

2.1 NetCDF climate data record (CDR) file name convention

The naming of the IASI Level 2 O_3 CDR products distributed on EUMETSAT data store follow the convention:

W_XX-EUMETSAT-Darmstadt,HYPERSPECT+SOUNDING,METOPX+O3+IASI_C_EUMP_ DateAndTimeStart _ DateAndTimeEnd _eps_r_l2_version.nc

where:

- W = For all products
- XX-EUMETSAT-Darmstadt = Location Identifier
- HYPERSPECT+SOUNDING = Data designator
- METOPX+O3+IASI = Free description: satellite (with X = A or B)+product+instrument
- C = For all products
- EUM**P** = Originator code for Operational (EUMETSAT **P**olar)
- DateAndTimeStart and DateAndTimeEnd are written in the form: YYYYMMDDhhmmssZ

with YYYYMMDD = the UTC year, month and day of the data start and end sensing times. hhmmss = the UTC hour, minute, second of the data start and end sensing times.

- eps = Native format
- r = reprocessing
- l2 = Level of data
- version = release version

2.2 CDR file size estimate

The size of the O_3 CDR files is on average 35 MB with ~14 orbits per day per instrument, with a total size of around 490 MB/day/instrument or 180 GB/year/instrument or 360 GB/year for the two instruments.

2.3 Description of the content of the netCDF file

The IASI L2 O_3 CDR netCDF files include FORLI-O_3 variables, and auxiliary variables (mainly meteorological) used to reconstruct atmospheric pressure profiles associated with O_3 observations. To optimize computing resources, a selection of IASI observations is made, prioritizing among the clear pixels. As a result, only about one observation in three or four is processed.

First we give an example of the file's global attributes. Table 1 details dimensions of FORLI-O_3 and auxiliary variables. In Tables 2 and 4 we list FORLI-O_3 variables and auxiliary variables, respectively. Table 3 describes the retrieval error flags combined in o3_bdiv.

```
// global attributes:
:creator_name = "EUMETSAT" ;
:creator_url = "http://www.eumetsat.int" ;
:creator_email = "ops@eumetsat.int" ;
:institution = "EUMETSAT" ;
:Conventions = "CF-1.7" ;
:Metadata_Conventions = "Unidata Dataset Discovery v1.0" ;
```

:data_format_type = "NetCDF-4 classic model" ;
:producer_agency = "EUMETSAT" ;
:platform = "M0X" ; with X = 2 for METOP-A or 1 for METOP-B
:platform_type = "spacecraft" ;
:sensor = "IASI" ;
:processing_level = "02" ;
:spacecraft_id = "M0X" ; with X = 2 for METOP-A or 1 for METOP-B
:processor_major_version = "6" ;
:product_minor_version = "5" ;
:format_major_version = "11" ;
:format_minor_version = "0" ;
:orbit_start = "48195" ;
:orbit_end = "48196" ;
:start_orbit_number = 48195 ;
:end_orbit_number = 48196 ;
:orbit_semi_major_axis = 7.204494e+09f ;
:orbit_eccentricity = 0.00121f ;
:orbit_inclination = 98.686f ;
:orbit_perigee_argument = 75.809f ;
:orbit_right_ascension = 63.334f ;
:orbit_mean_anomaly = 284.378f ;
:x_position = 5123897.f ;
:y_position = -5061554.f ;
:z_position = 6550.077f ;
:x_velocity = -1169.753f ;
:y_velocity = -1162.231f ;
:z_velocity = 7355.053f ;
:rev_orbit_period = 6081.7f ;
:equator_crossing_longitude = -5061554.f ;
:summary = "This file contains the Release 1 IASI L2 reprocessed for one orbit. The reprocessing was done on Linux using an adapted version of the EUMETSAT operational algorithm V6.6. Until december 2016, the reprocessed Metop-A IASI L1C input data were used (doi:10.15770/EUM_SEC_CLM_0014), after this date and for Metop-B the operational IASI L1c were used; this is to produce an homogeneous CDR. ERA5 were used as auxiliary model data";
:processing_mode = "R" ;
:start_sensing_data_time = "2022-01-01T00:56:53Z" ;
:end_sensing_data_time = "2022-01-01T02:41:57Z" ;
:start_sensing_data_time_theoretical = "2022-01-01T00:57:00Z" ;
:end_sensing_data_time_theoretical = "2022-01-01T02:42:00Z" ;
:production_date_time_start = "2023-02-22T18:44:32Z" ;
:production_date_time_end = "2023-02-22T18:44:33Z" ;
:equator_crossing_date_time = "2022-01-01T00:29:19Z" ;
:parent_name = "IASI_xxx_1C_M01_20220101005653Z_20220101024157Z_N_O_20220101014546Z" ;
:processing_centre = "EUM" ;
:source = "Metop-Y IASI" ; with Y = A or B
:platform_long_name = "Metop-Y" ; with Y = A or B
:project = "This data is provided as part of the EUMETSAT Satellite Application Facility on Atmospheric Composition Monitoring service, AC-SAF" ;
:id = "DOI: 10.15770/EUM_SAF_AC_0051" ;
:history = "Release 1" ;
:title = "IASI O3 CDR Release 1" ;
:title_short_name = "IASI O3 CDR" ;
:keywords = "IASI O3 CDR Climate" ;

Table 1: Dimensions of FORLI-O_3 and auxiliary variables

Dimension name	Dimension value	Dimension description
along_track	depends on the files	number of IASI scanlines included in the files
across_track	120	number of IASI pixels per scanline
nlt	101	number of vertical levels in temperature profiles
nlq	101	number of vertical levels in humidity profiles
nl_o3	41	number of vertical layers in O3 profiles
neva_o3	21	number of main eigenvalues of the sensitivity matrix
neve_o3	861	number of main eigenvectors of the sensitivity matrix

Table 2: Description of FORLI-O_3 variables in the netCDF file

Variable name in CDR O_3 product	Dimensions	Variable description and unit	Variable name in NRT O_3 product	Units
o3_cp_o3_a	along_track, across _track, nl_o3	A-priori partial columns for O3 on each retrieved layer between O3 partial layer heights given in forli_layer_heights_o3 variable	O3_CP_O3_A	molecules/ cm^2
o3_x_o3	along_track, across _track, nl_o3	Scaling vector multiplying the a-priori O3 vector in order to define the retrieved O3 vector on each retrieved layer between O3 partial layer heights given in forli_layer_heights_o3 variable	O3_X_O3	N/A
o3_nfitlayers	along_track, across _track	Number of layers actually retrieved	O3_NFITLAY ERS	N/A
o3_nbr_values	along_track	Number of O3 profiles retrieved in scanline	O3_NBR	N/A
o3_npca	along_track, across _track	Number of vectors describing the characterization matrices	O3_NPCA	N/A
o3_h_eigenval ues	along_track, across _track, neva_o3	Main eigenvalues of the sensitivity matrix	O3_H_EIGEN VALUES	N/A
o3_h_eigenve ctors	along_track, across _track, neve_o3	Main eigenvectors of the sensitivity matrix	O3_H_EIGEN VECTORS	N/A

o3_qflag	along_track, across _track	General quality flag of air partial columns on each retrieved layer (= 1 for the valuable pixels, to use with caution; = 0 for the remaining pixels that we recommend not to use)	O3_QFLAG	N/A
o3_bdiv	along_track, across _track	Retrieval flags	O3_BFIV_LO and O3_BDIV_HI	N/A
o3_cp_air	along_track, across_track, nl_o3	Air partial columns on each retrieved layer between O3 partial layer heights given in forli_layer_heights_o3 variable	O3_CP_AIR	molecules/ cm^2
forli_layer_heights_o3	nl_o3	O3 partial layer heights: the bottom height of the layer; 0 is understood as the altitude of the surface and the top of the atmosphere is at 60 km		m

In Table 2, o3_qflag is a single code assessing the quality of the retrieved profiles following the retrieval error flags o3_bdiv, as described in Table 3 below. o3_qflag is a FORLI- O_3 output, see Section 5.3.1.

Please note that the units of the variables a priori and air partial columns are molecules/cm^2, this is different from the IASI O_3 NRT product where the units of these variables are moles/cm^2.

Table 3: Potential processing and inputs errors and diagnostics on the retrieval of FORLI-O_3 (combined in 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	
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	

o3_bdiv is built by adding quality indicators associated to each IASI observation and to O_3 retrieval. As L1C and L2 input data were reprocessed, FORLI-O_3 results included in CDR netCDF files could be perceptibly different to FORLI-O_3 results included in NRT BUFR files. These differences can also affect o3_bdiv values.

Table 4: Description of auxiliary variables

Variable name in CDR O_3 product	Dimensions	Variable description and unit
atmospheric_temperature	along_track, across_track, nlt	Atmospheric temperature (for 120 IFOV with up to 101 vertical levels, in K)
atmospheric_water_vapor	along_track, across_track, nlq	Atmospheric water vapour (for 120 IFOV with up to 101 vertical levels, in kg/kg)
fg_atmospheric_temperature	along_track, across_track, nlt	A-priori atmospheric temperature profile (for 120 FOV with up to 101 vertical levels, in K)

fg_atmospheric_water_vapor	along_track, across_track, nlq	A-priori water vapour (for 120 FOV with up to 101 vertical levels, in kg/kg)
fg_surface_temperature	along_track, across_track	A-priori surface temperature (for 120 FOV, in K)
flag_daynit	along_track, across_track	Discrimination between day and night (0: day, 1: night, 2: twilight)
flag_landsea	along_track, across_track	Specifies surface type (0: water, 1: land low, 2: land high, 3: land water low, 4: land water high)
lat	along_track, across_track	Latitude
lon	along_track, across_track	Longitude
pressure_levels_humidity	nlq	Pressure levels on which atmospheric humidity profiles are retrieved (Pa)
pressure_levels_temp	nlt	Pressure levels on which atmospheric temperature profiles are retrieved (Pa)
record_start_time	along_track	Observation time at the start of the scanline (in seconds since 01/01/2000 at 00:00:00)
record_stop_time	along_track	Observation time at the end of the scanline (in seconds since 01/01/2000 at 00:00:00)
satellite_azimuth	along_track, across_track	angular relation for the earth view: satellite azimuth in degrees
satellite_zenith	along_track, across_track	angular relation for the earth view: satellite zenith in degrees
solar_azimuth	along_track, across_track	angular relation for the earth view: solar azimuth in degrees
solar_zenith	along_track, across_track	angular relation for the earth view: solar zenith in degrees
surface_pressure	along_track, across_track	Surface pressure (Pa)
surface_temperature	along_track, across_track	Surface temperature (for 120 IFOV, in K)
surface_z	along_track, across_track	Altitude of surface (m)

Usual FORLI-O_3 products have to be reconstructed/calculated from the fields mentioned in Table 2, see Section 5.

3. THE FORLI-O_3 product

3.1 Product description

The product FORLI-O_3 includes several variables, described above 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 top of the atmosphere (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** (‘o3_h_eigenvalues' and 'o3_h_eigenvectors'). Each retrieval has also associated retrieval flags.

Note that the retrievals are performed on the basis of the *a priori* partial columns (o3_cp_o3_a), which are scaled individually using a *multiplication factor* (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.

3.2 How to get the FORLI-O_3 products I need?

Table 5: FORLI-O_3 products that can be obtained from the O_3 CDR netCDF files.

FORLI-O_3 products	**Notation**	**How to get/calculate it?**
O_3 profile (molecules.cm^{-2})	o3_cp_o3	see Section 3.2.1, Eq 1
O_3 profile (VMR)	o3_vmr_o3	see Section 3.2.1, Eq 2
O_3 total column (molecules.cm^{-2})	o3_tc	see Section 3.2.1, Eq. 3
A priori profile (molecules.cm^{-2})	o3_cp_o3_a	Variable in netCDF file.
A priori profile (VMR)	o3_vmr_o3_a	See Section 3.2.3.2, Eq 10
Averaging Kernel matrix in scaling factor	A	see Section 3.2.2, Eq.6
Averaging Kernel matrix in partial column	A_{PC}	see Section 3.2.3.1, Eq. 9
Averaging Kernel matrix in VMR	A_{VMR}	see Section 3.2.3.2, Eq. 12
Total column averaging kernel vector	k	See Section 3.2.3.3, 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 3.2.3.3, Eq. 14
Relative error profile (relative to the retrieved O_3 profile in molecules.cm^{-2} or VMR)	σ	See Section 3.2.2, Eq. 7
Pressure levels (Pa)	p	See Section 5.2.3.4, Eq. 16 to 18

3.2.1 *Reconstruction of the O_3 profile and calculation of the total column*

The final **partial column profile** (molecules.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** (molecules.cm^{-2}) is obtained by summing the partial columns defined in Eq (1) on all retrieved layers:

$$cp\_tc = \sum_i \; o3\_cp\_o3_i \tag{3}$$

The total (or partial columns) can be similarly expressed in moles.cm^{-2} by dividing the values in molecules.cm^{-2} by 6.02214076x10^{+23}, the Avogadro constant.

3.2.2 *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. Typical compression rates are of about 4 for O_3. 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);
- S_a, the *a priori* variance-covariance matrix;
- $\hat{S}$, the posterior variance-covariance matrix;
- *A*, the averaging kernels matrix;
- and diag constructs a diagonal matrix the elements of which are given by the parameter vector.

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 v 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 4.1. S_a is also provided online on the EUMETSAT website (https://navigator.eumetsat.int/product/EO:EUM:DAT:METOP:IASIL2OZO/print, Ressources).

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 molecules.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.

3.2.3 Unit conversions

All computations made in Section 3.2.2 were done in the unitless space of the multiplication factor. Users wishing to change the unit space should apply the following conversion rules:

3.2.3.1 Partial columns

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

$$\hat{S}_{PC} = diag(o3\_cp\_o3\_a)\ \hat{S}\ diag(o3\_cp\_o3\_a) \tag{8}$$
$$A_{PC} = diag(o3\_cp\_o3\_a)A\ diag(o3\_cp\_o3\_a)^{-1} \tag{9}$$

3.2.3.2 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:

$$o3\_vmr\_o3\_a_i = o3\_cp\_o3\_a_i / o3\_cp\_air_i \quad \forall i \tag{10}$$
$$\hat{S}_{VMR} = diag(o3\_vmr\_o3\_a)\ \hat{S}\ diag(o3\_vmr\_o3\_a) \tag{11}$$
$$A_{VMR} = diag(o3\_vmr\_o3\_a)A\ diag(o3\_vmr\_o3\_a)^{-1} \tag{12}$$

3.2.3.3 Total columns

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

$$k \;\; = \left(k_1\ \ k_2\ \ \ldots\ \ k_{O3\_NFITLAYERS}\right),$$

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 on the total column is then calculated as σ_{TC}

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

3.2.3.4 Building of vertical pressure profiles associated with FORLI-O_3 products

Temperature and humidity vertical profiles extracted from the IASI L2 O_3 CDR product 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 O_3 CDR product.

From temperature and humidity vertical profiles, available in the CDR netcdf file, the correspondence between altitude and pressure could be calculated by iterating from the surface to the top of the atmosphere. When "atmospheric_temperature" profile is set to filling values, we replace "atmospheric_temperature" and "atmospheric_water_vapor" profiles by "fg_atmospheric_temperature" and "fg_atmospheric_water_vapor" profiles. The assumptions on the surface characteristics are:

surface altitude = z_0 ("surface_z", from CDR netCDF files)
surface pressure = p_0 ("surface_pressure" from CDR netCDF files)
surface temperature = T_o, extrapolation of the temperature profile T at the surface pressure ("atmospheric_temperature" or "fg_atmospheric_temperature" from CDR netCDF files)
surface humidity = q_o, first level of the humidity profile q ("atmospheric_water_vapor" or "fg_atmospheric_water_vapor" from CDR netCDF files)

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

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

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):

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

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

We obtain the altitude profile corresponding to the CDR “(fg_)atmospheric_temperature” and “(fg_)atmospheric_water_vapor” products.
Then we can extract the pressure levels associated to FORLI-O_3 product from the pressure vertical profile by using a cubic spline interpolation.

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

3.3 Using the product

3.3.1 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 not used, 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
- -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, we recommend using the data with o3_qflag equal to 1 and DOFS value higher than 2. DOFS values lower than 2 are mainly associated with bad quality data in Antarctic region [RD7].

3.4 Accuracy of the product

The accuracy of the product is given in terms of threshold, target and optimal values in Table 6 below. This information is taken from the Product Requirements Document [AD3]. The product performance is given in the Validation Report of this product.

Table 6: Accuracy of the FORLI-O_3 product

	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).

3.5 Validation of the product

A study conducted within the framework of the TOAR-II project, aimed to deepen the understanding of global tropospheric ozone spatiotemporal variability and trends, using the ozone Climate Data Record (CDR) from the IASI/Metop (IASI-CDR). The research focused on two main objectives: evaluating the quality and consistency of the IASI-CDR O3 product and investigating the spatiotemporal variability and long-term trends in ozone [RD8].

Key findings are summarized as follows:

- A comparison with CrIS-TROPESS data shows excellent agreement for total ozone (biases < 1.2%, correlations > 0.97) and good agreement for tropospheric ozone (biases 10–12%, correlations 0.77–0.91). However, systematic overestimations in CrIS tropospheric ozone, particularly at high northern and southern mid-latitudes, indicate the need for further investigation.
- When compared with ozonesonde data, IASI-CDR profiles generally capture ozone distribution features well, but tend to underestimate tropospheric and stratospheric ozone, and overestimate UTLS ozone. The IASI-CDR product underestimates the tropospheric ozone column, with biases ranging from -2% in the tropics to -10% in mid- and high-latitudes.
- A regional drift is found in the IASI-SONDE bias over Europe (-0.12 ± 0.05%/yr), primarily linked to the Payerne station. On a global scale, no drift is found, and excluding Payerne, no drift is observed over Europe. Further investigation of this drift is needed to ensure consistency in long-term ozone trend assessments.

3.6 Product dissemination and archiving

The IASI CDR Level 2 products are disseminated to users through EUMETSAT Data Store [RD6]. The data are disseminated in netCDF format. A full description of the IASI O_3 CDR Level 2 netCDF content is given in Section 2.

3.7 Product ordering

Access to this data record is granted to all users without charge but accepting the EUMETSAT Data Policy provided in the corresponding EUMETSAT webpage: https://www.eumetsat.int/legal-framework/data-policy

To access data, you need to register with the EUMETSAT Data Centre. When registered, you can order the data through a written request send to EUMETSAT's helpdesk.

3.7.1 Register with the Data Centre

Do this to register with the EUMETSAT Data Centre:
- Register in the EUMETSAT EO-Portal (https://eoportal.eumetsat.int) by clicking on the New User
- Create New Account tab;
- After finalisation of the registration process, an e-mail is sent to the e-mail address entered in the registration. Click the confirmation link in the e-mail to activate your account;
- Login and subscribe to the Data Centre Service by going to the Service Subscription Tab and selecting Data Centre Service. Follow instructions issued from the web page to add needed information.

3.7.2 Order Data

The data record described in this product user guide can also be ordered via the EUMETSAT User Service Helpdesk in Darmstadt, Germany. Please send a written request to the helpdesk, email ops@eumetsat.int, indicating the data record that you want to order including its Digital Object Identifier (DOI) number: 10.15770/EUM_SAF_AC_0051.

4. Appendices

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

```
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6.10373820e-02 5.31293920e-02 4.59736110e-02 3.83454520e-02 6.25738742e-03;
-6.40761030e-03 -6.90247320e-03 4.04730860e-03 1.19576800e-02 1.56237740e-02 1.55100830e-02
1.13775450e-02 -1.93553110e-03 -3.41123160e-02 -8.49125980e-02 -1.18963580e-01 -1.31989310e-01 -
1.39691680e-01 -1.50351040e-01 -1.60122780e-01 -1.66990560e-01 -1.64802460e-01 -1.50897170e-01 -
1.27131960e-01 -9.74773940e-02 -7.08074380e-02 -4.72512370e-02 -2.49716340e-02 -4.86196780e-03
1.35557610e-02 3.06573060e-02 4.56521770e-02 5.84666280e-02 6.86961320e-02 7.56843350e-02
7.99435270e-02 8.15250150e-02 8.05258460e-02 7.67178190e-02 7.13881390e-02 6.50653870e-02
5.85296280e-02 5.10681430e-02 4.42795260e-02 3.70140980e-02 6.02865638e-03;
-5.12864270e-03 -5.31118480e-03 5.15381810e-03 1.24151060e-02 1.57230480e-02 1.55000460e-02
1.16793140e-02 -6.05837780e-04 -3.02759950e-02 -7.72204280e-02 -1.08389630e-01 -1.20187480e-01 -
1.27408800e-01 -1.37622700e-01 -1.47020220e-01 -1.53543870e-01 -1.51533140e-01 -1.38548470e-01 -
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7.40838020e-02 7.55946300e-02 7.47709380e-02 7.13881390e-02 6.66062390e-02 6.08910040e-02
5.49383010e-02 4.81066880e-02 4.18641180e-02 3.51532600e-02 5.86766152e-03;
-3.89231390e-03 -3.78424280e-03 6.05647540e-03 1.25416940e-02 1.54052920e-02 1.50409740e-02
1.15500350e-02 4.27512070e-04 -2.63884050e-02 -6.89423180e-02 -9.68248460e-02 -1.07195110e-01 -
1.13799120e-01 -1.23400130e-01 -1.32260580e-01 -1.38338230e-01 -1.36513950e-01 -1.24582920e-01 -
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6.72745380e-02 6.86618080e-02 6.79966250e-02 6.50653870e-02 6.08910040e-02 5.58870260e-02
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1.00968630e-01 -1.09861610e-01 -1.18070230e-01 -1.23551680e-01 -1.21804390e-01 -1.10907300e-01 -
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1.01975480e-02 1.43039060e-03 -1.95120860e-02 -5.29457550e-02 -7.41277180e-02 -8.15191680e-02 -
8.66769670e-02 -9.46554480e-02 -1.02051060e-01 -1.06877320e-01 -1.05297520e-01 -9.56169360e-02 -
7.96258660e-02 -5.97982540e-02 -4.20097760e-02 -2.64632850e-02 -1.19200510e-02 9.92673720e-04
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5.25514450e-02 5.35683220e-02 5.31293920e-02 5.10681430e-02 4.81066880e-02 4.45674820e-02
4.08654610e-02 3.65401390e-02 3.26104890e-02 2.82883620e-02 6.37213622e-03;
-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];
```

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

```
------------------------------------------------------------------------------
##########################################################################
#        Reading routine in Python to reconstruct H, S and A         #
##########################################################################

"""
From one single L2 O3 CDR netcdf file, this script reads variables, deletes observations
with latitude and longitude out of normal range, and, for valuable observations,
reconstructs matrices and estimates retrieval errors.

Usage : python -Wignore reconstruct_matrices_PUM.py

"""

# metadata information
__date__ = "21 March 2025"
__author__ = "J. Hadji-Lazaro"
__copyright__ = "Copyright 2025, LATMOS"
__organization__ = "LATMOS/CNRS/UVSQ/SU"
__license__ = "GPL"
__maintainer__ = "J. Hadji-Lazaro"
__email__ = "juliette.hadji-lazaro@latmos.ipsl.fr"

import sys
import numpy as np
import pandas as pd
from netCDF4 import Dataset
import csv

# read a priori variance-covariance matrix, provided in section 4.1
Sa_O3_init=pd.read_csv('Sa_O3',sep=' ',header=None,index_col=False)
Sa_O3=Sa_O3_init.values
del(Sa_O3_init)

# read one single L2 O3 CDR netcdf file and delete observations for which latitudes and longitudes
# do not have valid values
netcdf_inputfile='PATH_TO_O3_CDR_FILES/W_XX-EUMETSAT-
Darmstadt,HYPERSPECT+SOUNDING,METOPX+O3+IASI_C_EUMP_YYYYMMDDhhmmssZ_YYYY
MMDDhhmmssZ_eps_r_l2_0100.nc'
print(netcdf_inputfile)
data = Dataset(netcdf_inputfile, 'r', format='NETCDF4')
along_track=data.dimensions['along_track'].size
print(along_track)
across_track=data.dimensions['across_track'].size
print(across_track)
nlo3=data.dimensions['nl_o3'].size
print(nlo3)
nevao3=data.dimensions['neva_o3'].size
print(nevao3)
lat=data.variables['lat']
size_lat=list(np.shape(lat))
lat=np.reshape(lat,size_lat[0]*size_lat[1])
```

```
lon=data.variables['lon']
lon=np.reshape(lon,size_lat[0]*size_lat[1])
lon=np.delete(lon,np.where(abs(lat)>90.))
gqf=data.variables['co_qflag']
gqf=np.reshape(gqf,size_lat[0]*size_lat[1])
gqf=np.delete(gqf,np.where(abs(lat)>90.))
prior=data.variables['o3_cp_o3_a']
prior=np.reshape(prior,(size_lat[0]*size_lat[1],nlo3))
prior=np.delete(prior,np.where(abs(lat)>90.),axis=0)
air=data.variables['o3_cp_air']
air=np.reshape(air,(size_lat[0]*size_lat[1],nlo3))
air=np.delete(air,np.where(abs(lat)>90.),axis=0)
scalfac=data.variables['o3_x_o3']
scalfac=np.reshape(scalfac,(size_lat[0]*size_lat[1],nlo3))
scalfac=np.delete(scalfac,np.where(abs(lat)>90.),axis=0)
nfitlay=data.variables['o3_nfitlayers']
nfitlay=np.reshape(nfitlay,size_lat[0]*size_lat[1])
nfitlay=np.delete(nfitlay,np.where(abs(lat)>90.))
npca=data.variables['o3_npca']
npca=np.reshape(npca,size_lat[0]*size_lat[1])
npca=np.delete(npca,np.where(abs(lat)>90.))
eve=data.variables['o3_h_eigenvectors']
eve=np.reshape(eve,(size_lat[0]*size_lat[1],nevao3*nlo3))
eve=np.delete(eve,np.where(abs(lat)>90.),axis=0)
eva=data.variables['o3_h_eigenvalues']
eva=np.reshape(eva,(size_lat[0]*size_lat[1],nevao3))
eva=np.delete(eva,np.where(abs(lat)>90.),axis=0)
lat=np.delete(lat,np.where(abs(lat)>90.))
data.close()

# for each observation, calculation of the ratio between the minimum and maximum values of the
# scale factor profile (scalfac) above sea surface level
scaltemp=np.tile(np.nan,(len(lat),41))
for i in range(len(lat)) :
    if nfitlay[i]>-1 :
        scaltemp[i,0+(41-nfitlay[i]):41]=scalfac[i,0+(41-nfitlay[i]):41]
scalmin=np.nanmin(scaltemp,1) # NaN if all elements of scaltemp are NaN
scalmax=np.nanmax(scaltemp,1) # NaN if all elements of scaltemp are NaN
ratio=np.divide(scalmax,scalmin) # NaN if scalmin and/or scalmax is NaN

ratio_nan=np.isnan(ratio)
ratio_inf=np.isinf(ratio)
# detection of NaN in scalfac
nan_in_scal_day=np.isnan(scalfac)
depist_nan=np.tile(0,(len(lat)))
depist_nan=np.where(nan_in_scal_day.sum(axis=1) > 0, 1, depist_nan)
# detection of Inf in scalfac
inf_in_scal_day=np.isinf(scalfac)
depist_inf=np.tile(0,(len(lat)))
depist_inf=np.where(inf_in_scal_day.sum(axis=1) > 0, 1, depist_inf)
# detection of zeros in scalfac
zeros_in_scalfac=np.tile(0,(len(lat),41))
zeros_in_scalfac[scalfac==0]=1
depist_zeros_scalfac=np.tile(0,(len(lat)))
```

```
depist_zeros_scalfac=np.where(zeros_in_scalfac.sum(axis=1) > 0, 1, depist_zeros_scalfac)
# detection of values between 650000 and 660000 in scalfac
outliers_650k_in_scal_day=np.tile(0,(len(lat),41))
outliers_650k_in_scal_day[(scalfac>650000.)&(scalfac<660000.)]=1
depist_outliers_650k=np.tile(0,(len(lat)))
depist_outliers_650k=np.where(outliers_650k_in_scal_day.sum(axis=1) > 0, 1, depist_outliers_650k)
# detection of filling values above surface level in scalfac (values higher than 9.96e36 in scaltemp, scalfac
# above sea surface level)
outliers_in_scal_day=np.tile(0,(len(lat),41))
outliers_in_scal_day[scaltemp>9.96e36]=1
depist_outliers=np.tile(0,(len(lat)))
depist_outliers=np.where(outliers_in_scal_day.sum(axis=1) > 0, 1, depist_outliers)
# detection of scalfac profiles lower than 1e-5
depist_profils_inf1=np.tile(0,(len(lat)))
depist_profils_inf1=np.where(scalmin <= 1.e-5, 1, depist_profils_inf1)
# detection of zeros in prior
zeros_ds_prior=np.tile(0,(len(lat),41))
zeros_ds_prior[prior==0]=1
depist_zeros_prior=np.tile(0,(len(lat)))
depist_zeros_prior=np.where(zeros_ds_prior.sum(axis=1) > 0, 1, depist_zeros_prior)
# detection of zeros in air profile
zeros_ds_air_prof=np.tile(0,(len(lat),41))
zeros_ds_air_prof[air==0]=1
depist_zeros_air=np.tile(0,(len(lat)))
depist_zeros_air=np.where(zeros_ds_air_prof.sum(axis=1) > 0, 1, depist_zeros_air)

# conversion in moles/m2 and replacement of filling values by NaN
prior=np.where(prior > 65535., prior/6.02214086e+19, np.nan)
air=np.where(air > 65535., air/6.02214086e+19, np.nan)
scalfac=np.where(scalfac < 9.96e+36, scalfac, np.nan)
fit=prior*scalfac
coltot=np.nansum(fit,axis=1)

# detection of prior profiles including less "not NaN" values than the number of layers actually retrieved
(nfitlay)
prior_aberrant=np.tile(0,(len(lat),41))
prior_aberrant[~np.isnan(prior)]=1
depist_prior_aberrant=np.tile(0,(len(lat)))
depist_prior_aberrant=np.where((nfitlay > -1) & (prior_aberrant.sum(axis=1) < nfitlay), 1,
depist_prior_aberrant)

print('Errors estimation and matrices reconstruction')
#   initialisation of errors, averaging kernel matrix and dofs
fit_out=np.tile(np.nan,(len(lat),41))
coltot_out=np.tile(np.nan,(len(lat)))
ERROR_PROF=np.tile(np.nan,(len(lat),41))
ERROR_COLTOT=np.tile(np.nan,(len(lat)))
AVK=np.tile(np.nan,(len(lat),41,41))
dofs=np.tile(np.nan,(len(lat)))
for i in range(len(lat)) :
    i=int(i)
# tests to avoid processing outliers
    if nfitlay[i] > -1 and gqf[i] > -1 and ratio[i] != 1 and ratio_nan[i] == 0 and ratio_inf[i] == 0 and
depist_nan[i] == 0 and depist_inf[i] == 0 and depist_zeros_scalfac[i] == 0 and depist_zeros_prior[i] == 0
```

```
and depist_zeros_air[i] == 0 and depist_outliers_650k[i] == 0 and depist_outliers[i] == 0 and
depist_prior_aberrant[i] == 0 and depist_profils_inf1[i] == 0 and np.sum(eva[i,range(npca[i])]) == npca[i]:
        fit_out[i,:]=fit[i,:]
        coltot_out[i]=coltot[i]
#   matrices reconstruction + errors estimation
        tmp_eve=eve.take(i,axis=0)
        tmp_eve2=tmp_eve.take(range(0,int(nfitlay[i])*int(npca[i])))
        transp_nu=np.reshape(tmp_eve2,(int(npca[i]),int(nfitlay[i])))
        del(tmp_eve)
        del(tmp_eve2)
        nu=np.transpose(transp_nu)
        tmp_eva=eva.take(i,axis=0)
        tmp_eva2=tmp_eva.take(range(0,int(npca[i])))
        dia_lambda=np.diag(tmp_eva2)
        del(tmp_eva)
        del(tmp_eva2)
        H1=nu.dot(dia_lambda)
        H=H1.dot(transp_nu)
        del(H1)
        Sa=Sa_O3.take(range(41-int(nfitlay[i]),41),axis=1)
        Sa=Sa.take(range(41-int(nfitlay[i]),41),axis=0)
        inv_Sa=np.linalg.inv(Sa)
        S=np.linalg.inv(H+inv_Sa)
        ERROR_PROF1=np.divide(np.sqrt(np.diag(S)),scalfac[i,range(41-int(nfitlay[i]),41)])
        ERROR_PROF[i,range(41-int(nfitlay[i]),41)]=ERROR_PROF1
        S_CP1=np.diag(prior[i,range(41-int(nfitlay[i]),41)]).dot(S)
        S_CP=S_CP1.dot(np.diag(prior[i,range(41-int(nfitlay[i]),41)]))
        del(S_CP1)
        ERROR_COLTOT[i]=np.sqrt(np.sum(np.sum(S_CP)))/np.sum(fit[i,range(41-int(nfitlay[i]),41)])
        del(S_CP)
        AVK_SF=S.dot(H)
        del(H)
        del(S)
        AVK_CP1=np.diag(prior[i,range(41-int(nfitlay[i]),41)]).dot(AVK_SF)
        AVK_CP=AVK_CP1.dot(np.linalg.inv(np.diag(prior[i,range(41-int(nfitlay[i]),41)])))
        del(AVK_CP1)
        dofs[i]=np.sum(np.diag(AVK_CP))
        AVK[i,41-int(nfitlay[i,]):,41-int(nfitlay[i]):]=AVK_CP
        del(AVK_CP)

print('Writing in output files')

mat_zip=np.hstack((lat[:,None],lon[:,None],gqf[:,None],nfitlay[:,None],6.02214086E+19*fit_out[:,:],ERRO
R_PROF[:,:],6.02214086E+19*coltot_out[:,None],ERROR_COLTOT[:,None],dofs[:,None]))

outputfile="profiles_and_column.out"
output_id=open(outputfile,'w')
output_writer = csv.writer(output_id,delimiter=' ')
output_writer.writerows(mat_zip)
output_id.close()

AVK_zip=np.vstack(AVK[:,:,:])
AVKfile="AVK.out"
AVK_id=open(AVKfile,'w')
```

```
AVK_writer = csv.writer(AVK_id,delimiter=' ')
AVK_writer.writerows(AVK_zip)
AVK_id.close()
```

The script source (reconstruct_matrices_PUM.py or Clean_and_Reconstruct_O3_matrix_final.py in notebook version), the *a priori* variance-covariance matrix S_a (Sa_O3) and examples of output files are available at the address https://owncloud.latmos.ipsl.fr/index.php/s/qjFiL6GnpFGdmkP. The *_outliers.out files are output files associated with W_XX-EUMETSAT-Darmstadt,HYPERSPECT+SOUNDING,METOPB+O3+IASI_C_EUMP_20220222121200Z_20220222130559Z_eps_r_l2_0100.nc. Profiles_and_column.out and AVK.out are output files associated with W_XX-EUMETSAT-Darmstadt,HYPERSPECT+SOUNDING,METOPB+O3+IASI_C_EUMP_20220222145400Z_20220222163255Z_eps_r_l2_0100.nc.

4.3 IASI-FORLI retrieval algorithm

4.3.1 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].

4.3.2 FORLI overview

FORLI (Fast Optimal/Operational Retrievals on Layers for IASI) is a radiative transfer model based on precalculated look-up tables (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].

Information on how to use the NRT O_3 product can be found in the NRT O_3 PUM [AD2].