The EUMETSAT Network of Satellite Application Facilities

O3M SAF
Ozone and Atmospheric Chemistry Monitoring

PRODUCT USER MANUAL

Near real-time IASI CO

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DOCUMENT STATUS SHEET

Issue	Date	Modified items/Reason for change
1.1	18/12/2015	The document has been modified according to the RID. Section 4 and 5 has been switched and completed.
1.2	08/12/2016	Section 5.3.1 regarding CO_QFLAG has been modified.

TABLE OF CONTENTS

1. INTRODUCTION

1.1 Purpose and scope

This document is the Product User Manual for the Near Real Time IASI CO profiles retrieved within the context of the Satellite Application Facility on Ozone and Atmospheric Chemistry Monitoring (O3M SAF) Second Continuous Development and Operations Phase (CDOP-2). This document gives a brief overview on the IASI retrieval algorithm and explains how to use and interpret the IASI CO profiles.

This document has been written as FORLI-CO v20140922 was running at EUMETSAT.

1.2 Acronyms

O3M SAF: Ozone and Atmospheric Composition Monitoring Satellite Application Facility
CDOP-2: Second Continuous Development and Operations Phase (CDOP-2)
EUMETSAT: European Organisation for the Exploitation of Meteorological Satellites
EUMETCast: EUMETSAT multi-service data dissemination system
CAF: Central Application Facility at EUMETSAT
WMO: World Meteorological Organization
GTS: Global Telecommunication System
IASI: Infrared Atmospheric Sounding Interferometer
FORLI: Fast Optimal 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-CO Product Specification, Requirement And Assessment SAF/O3M/ULB/FORLICO_PSRA Issue 1, 21/01/2015

[AD3] Product Requirements Document SAF/O3M/FMI/RQ/PRD/001 Issue 1.6, 03/12/2014

[AD4] IASI CO validation report SAF/O3M/LATMOS/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] EUMETCast Dissemination facility
http://www.eumetsat.int/website/home/Data/DataDelivery/EUMETCast/index.html

2. INTRODUCTION TO EUMETSAT SATELLITE APPLICATION FACILITY FOR ATMOSPHERIC COMPOSITION AND UV RADIATION (O3M SAF)

2.1 Background

The need for atmospheric chemistry monitoring was first realized when severe loss of stratospheric ozone was detected over the Polar Regions. At the same time, increased levels of ultraviolet radiation were observed.

Ultraviolet radiation is known to be dangerous to humans and animals (causing e.g. skin cancer, cataract, immune suppression) and having harmful effects on agriculture, forests and oceanic food chain. In addition, the global warming - besides affecting the atmospheric chemistry - also enhances the ozone depletion by cooling the stratosphere. Combined, these phenomena have immense effects on the whole planet. Therefore, monitoring the chemical composition of the atmosphere is a very important duty for EUMETSAT and the world-wide scientific community.

2.2 Objectives

The main objectives of the O3M SAF is to process, archive, validate and disseminate atmospheric composition products (O_3, NO_2, SO_2, BrO, HCHO, H_2O), aerosol products and surface ultraviolet radiation products utilising the satellites of EUMETSAT. The majority of the O3M SAF products are based on data from the GOME-2 spectrometers onboard Metop-A and Metop-B satellites and some new products from the IASI mission: CO, SO_2, O_3 and HNO_3.

Another important task of the O3M SAF is the research and development in radiative transfer modelling and inversion methods for obtaining long-term, high-quality atmospheric composition products from the satellite measurements.

2.3 Product categories, timeliness and dissemination

Data products are divided in two categories depending on how quickly they are available to users:

Near real-time 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
  - O_3, NO_2, NO_2Tropo, CO, HNO_3, SO_2
- Near real-time ozone profiles
  - coarse and high-resolution
- 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 in two weeks after measurement and disseminated via dedicated web services at EUMETSAT, FMI and DLR.

- Offline trace gas columns
  - O_3, NO_2, NO_2Tropo, SO_2, BrO, HCHO, H_2O

- Offline ozone profiles
    - coarse and high-resolution
- Offline absorbing aerosol indexes
    - from main science channels and polarization measurement detectors
- Offline surface UV

More information about the O3M SAF project, products and services: http://o3msaf.fmi.fi/

O3M SAF Helpdesk: o3msaf@fmi.fi

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 CO PRODUCT

4.1 BUFR PDU file name convention

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

W_XX-EUMETSAT- Darmstadt,SOUNDING+SATELLITE,METOP*+IASI_C_EUMC_
*yyyymmdd*hhmmss_nnnnn_eps_o_cox_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

4.2 BUFR file size estimate

The size of the output may vary and is on average 850 KB 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 CO BUFR PDU file structure is summarised below. The FORLI-CO product is provided in the 10 last fields (in bold).

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

DATA DESCRIPTOR		NAME USED HEREAFTER
0-0-1007	SATELLITE IDENTIFIER	
0-0-1031	IDENTIFICATION OF ORIGINATING/GENERATING CENTRE	
0-25-060	SOFTWARE IDENTIFICATION	
0-0-2019	SATELLITE INSTRUMENTS	
0-0-2020	SATELLITE CLASSIFICATION	
0-0-4001	YEAR	
0-0-4002	MONTH	
0-0-4003	DAY	
0-0-4004	HOUR	
0-0-4005	MINUTE	
0-0-4006	SECOND	
0-0-5040	ORBIT NUMBER	
0-0-5041	SCAN LINE NUMBER	
0-0-5001	LATITUDE (HIGH ACCURACY)	

0-0-6001	LONGITUDE (HIGH ACCURACY)	
0-0-5043	FIELD OF VIEW NUMBER	
0-0-7024	SATELLITE ZENITH ANGLE	
0-0-5021	BEARING OR AZIMUTH (DEGREE TRUE)	
0-0-7025	SOLAR ZENITH ANGLE	
0-0-5022	SOLAR AZIMUTH (DEGREE TRUE)	
0-0-7007	HEIGHT (Surface altitude in meter)	
0-4-0242	**GENERAL RETRIEVAL QUALITY FLAG**	**CO_QFLAG**
0-4-0243	**RETRIEVAL FLAGS**	**CO_BDIV**
0-4-0244	**NUMBER OF VECTORS DESCRIBING THE CHAR. MATRICES**	**CO_NPCA**
0-4-0245	**NUMBER OF LAYERS ACTUALLY RETRIEVED**	**CO_NFITLAYERS**
0-4-0246	**NUMBER OF CO PROFILES RETRIEVED IN SCANLINE**	**CO_NBR**
0-4-0247	**AIR PARTIAL COLUMNS ON EACH RETRIEVED LAYER**	**CO_CP_AIR**
0-4-0248	**A-PRIORI PARTIAL COLUMNS FOR CO EN EACH RETRIEVED LAYER**	**CO_CP_CO_A**
0-4-0249	**SCAL. VEC. MULT. A-PRI. CO VEC. DEF. RETR. CO VEC.**	**CO_X_CO**
0-4-0250	**MAIN EIGENVALUES OF THE SENSITIVITY MATRIX**	**CO_H_EIGENVALUES**
0-4-0251	**MAIN EIGENVECTORS OF THE SENSITIVITY MATRIX**	**CO_H_EIGENVECTORS**

Usual FORLI-CO 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-CO products can be found in files distributed by EUMETCast called:
W_XX-EUMETSAT- Darmstadt,SOUNDING+SATELLITE,METOP*+IASI_C_EUMC_
*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

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

5. THE FORLI-CO PRODUCT

5.1 Product description

The product FORLI-CO includes several variables, described in Table 1 (bold) and in Table 2. The principal product is a vertical profile of CO provided on 18 layers, from the ground to 18 km with an additional layer from 18 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 CO EN EACH RETRIEVED LAYER" called hereafter *CO_CP_CO_A)*, which are scaled individually using a *multiplication factor* ("SCAL. VEC. MULT. A-PRI. CO VEC. DEF. RETR. CO VEC*"* called hereafter *CO*_X_*CO*). The multiplication factor equals therefore 1 at initial stage, is unit less, 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 *CO_CP_CO_A* is computed using ray tracing methods described in the ATBD [AD1], while *CO*_X_*CO* is retrieved using OEM method in a logarithmic space in order to avoid nonphysical negative values.

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

Name	**Description**	**Units**
CO_QFLAG	General quality flag	N/A
CO_BDIV	Retrieval flags	N/A
CO_NPCA	Number of vectors describing the characterization matrices	N/A
CO_NFITLAYERS	Number of layers actually retrieved; ≤ 19	N/A
CO_NBR	Number of CO profiles retrieved in scanline	N/A
CO_CP_AIR	Air partial column on each retrieved layer	molecules /cm2
CO_CP_CO_A	A priori partial columns for CO on each retrieved layer	molecules /cm2
CO_X_CO	Scaling vector multiplying the a priori CO vector in order to define the retrieved CO vector	N/A
CO_H_EIGENVALUES	Main eigenvalues of the sensitivity matrix	N/A
CO_H_EIGENVECTORS	Main eigenvectors of the sensitivity matrix	N/A

In Table 2 CO_QFLAG is meant to be a single code assessing the quality of the retrieved profiles following the retrieval error flags CO_BDIV, as described in Table 3 below. CO_QFLAG is not implemented for the moment (v20140922) and CO_BDIV is not correctly implemented (See the ‘IASI CO Validation Report’ [AD4]).

Table 3: Retrieval flags of FORLI-CO (CO_BDIV) used in the released data.

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

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

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

FORLI-CO products	Notation	How to get/calculate it?	From
CO profile (molecules/cm^2)	CO_CP_CO	see Section 5.2.1, Eq 1	cox
CO profile (VMR)	CO_VMR_CO	see Section 5.2.1, Eq 2	
CO total column (molecules/cm^2)	CO_TC	see Section 5.2.1, Eq. 3	
A priori profile (molecules/cm^2)	CO_CP_CO_A	Field "A-PRIORI PARTIAL COLUMNS FOR CO EN EACH RETRIEVED LAYER"	
A priori profile (VMR)	CO_VMR_CO_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 CO profile in molecules/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 CO 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.:

$$CO\_CP\_CO_i = CO\_CP\_CO\_A_i \times CO\_X\_CO_i \quad \forall i \tag{1}$$

Profile spans *CO_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:

$$CO\_VMR\_CO_i = CO\_CP\_CO_i \div CO\_CP\_AIR_i \quad \forall i \tag{2}$$

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

$$CO\_TC = \sum_i CO\_CP\_CO_i \tag{3}$$

The total (or partial columns) can be similarly expressed in kg m^{-2} by multiplying the values in molecules cm^{-2} by 4.65119×10^{-22}.

5.2.2 Reconstruction of the characterisation matrices

Averaging kernel, which is normally an asymmetric matrix (*CO_NFITLAYERS* × *CO_NFITLAYERS*), is compressed by using a principal component decomposition representation. A reduced subset of principal vectors (*CO_NPCA* out of *CO_NFITLAYERS*) of the sensitivity matrix, *H*, is retained in order to achieve a meaningful compression. Typical compression rates are of about 4 for CO. 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 (*CO_NFITLAYERS* × *CO_NPCA*);
- λ, the principal eigenvalues vector (*CO_NPCA* × *CO_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. CO_NFITLAYERS < 19), 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 *CO_H_EIGENVECTORS* linear entry properly reshaped, and eigenvalues vector λ is the *CO_H_EIGENVALUES* entry.

The *a priori* variance-covariance matrix S_a needed for the reconstruction is provided in Section 6.1. S_a is also provided online on EUMETSAT website (TBD).

Then the relative error profile can be calculated:

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

As it is relative to the retrieval, the relative error profile is the same for the retrieved CO 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.

5.2.3 Unit conversions

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

5.2.3.1 Partial columns

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

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

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 *CO_CP_AIR*. Hence conversions are given by:

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

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:

$k \;\; = (k_1 \;\; k_2 \;\; \dots \;\; k_{CO\_NFITLAYERS})$,
with $k_i = A_{1,i} + A_{2,i} + \dots + A_{CO\_NFITLAYERS,i}$, i=1 to CO_NFITLAYERS, (13)

The absolute total retrieval error on the total column is then calculated as σ_{TC}

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

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-CO 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:

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

where

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

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

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

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):

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

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-CO 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

CO_QFLAG is a quality assessment associated with the quality of FORLI retrieved CO total column. CO_QFLAG is a FORLI-CO output. It can be 2 (best quality), 1 (acceptable quality) or 0 (the rest).

CO_QFLAG=2 for the most reliable pixels, in other words the best quality pixels, *i.e.* when:

- DOFS > 0.5376,
- CO total column < 20 x 10^{18} molecules/cm^2,
- the flag AMP_NEGPC (negative retrieval for H_2O) is null
- **1.** flags AMP_NEGZ0, AMP_TSKIN, AMP_TDIFF, AMP_DESERT, AMP_ITERATIONS, AMP_SLOPE, AMP_CONTRAST, AMP_AVK, AMP_BIAS and AMP_RMS are null

  or

  2. total cloud cover ≤12% and flags AMP_NEGZ0, AMP_TDIFF, AMP_DESERT, AMP_ITERATIONS, AMP_SLOPE, AMP_CONTRAST, AMP_AVK, AMP_BIAS and AMP_RMS are null.

CO_QFLAG=1 for the valuable pixels, to use with caution, .*i.e.* when:

- DOFS > 0.5376,
- CO total column < 20 x 10^{18} molecules/cm^2,

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

For data validation or assimilation purposes, we recommend using the data with CO_QFLAG equal to 2. For specific studies, if more pixels are needed, CO_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 accuracy of the product is given in terms of threshold, target and optimal values in Table 5 below. This information is taken from the FORLI-CO product specification, requirement and assessment document [AD2] and is also given in the Product Requirements Document [AD3].

Table 5: Accuracy of the FORLI-CO product.

		Accuracy (%)			Spatial resolution	Spatial coverage	Cloud fraction	NRT
		Threshold	Target	Optimal				
Total column	*Standard*	25	12	5	IASI pixel	Global	< 25 %	< 3h
	Unusual	50	20	10				
Near-surface VMR	*Standard*	50	30	12	IASI pixel	Global	< 25 %	< 3h
	Unusual	150	100	12				
Layer-averaged VMR in free troposphere (1 km)		25	12	5	IASI pixel	Global	< 25 %	< 3h

5.5 Validation of the product

The validation of the FORLI-CO product is performed at LATMOS. The 'IASI CO validation report' [AD4] give some scientific validation results and assess the similitude between the products disseminated by EUMETCast and the products generated at ULB/LATMOS. Possible processing errors as well as abnormal behavior are noticed and checked.

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 [RD6] with a time lapse of two hours from sensing to delivery. The data are disseminated in WMO (BUFR) format. A full description of the IASI CO Level 2 BUFR content is given in Section 4.3.

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, either in EPS native, in BUFR or in NetCDF format.

6. APPENDICES

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

```
Sa['CO']=matrix([[+3.9650531E-01,+2.5280535E-01,+1.9817827E-01,+1.6509750E-
01,+1.4575962E-01,+1.3394338E-01,+1.2549382E-01,+1.1861376E-01,+1.0993634E-
01,+9.8773297E-02,+8.5791044E-02,+7.0830532E-02,+5.9056920E-02,+4.6892112E-
02,+3.6040621E-02,+2.7196075E-02,+2.0282477E-02,+1.6480811E-02,+1.2681867E-02],

[+2.5280535E-01,+2.1312735E-01,+1.7760667E-01,+1.5098094E-01,+1.3355103E-
01,+1.2313758E-01,+1.1514362E-01,+1.0878214E-01,+1.0160108E-01,+9.2449041E-
02,+8.1896901E-02,+6.8933915E-02,+5.7637855E-02,+4.5622891E-02,+3.5272658E-
02,+2.7180976E-02,+2.0831196E-02,+1.7531716E-02,+1.4114632E-02],

[+1.9817827E-01,+1.7760667E-01,+1.6324326E-01,+1.4154247E-01,+1.2598168E-
01,+1.1645555E-01,+1.0885072E-01,+1.0253117E-01,+9.5641950E-02,+8.7176116E-
02,+7.7261109E-02,+6.4852199E-02,+5.3756843E-02,+4.2089189E-02,+3.2444706E-
02,+2.5153707E-02,+1.9418228E-02,+1.6626404E-02,+1.3696698E-02],

[+1.6509750E-01,+1.5098094E-01,+1.4154247E-01,+1.3055180E-01,+1.1882531E-
01,+1.1036372E-01,+1.0351414E-01,+9.7197261E-02,+9.0595067E-02,+8.2420077E-
02,+7.3115010E-02,+6.1147391E-02,+5.0348259E-02,+3.9108593E-02,+2.9978290E-
02,+2.3214689E-02,+1.7877493E-02,+1.5401913E-02,+1.2795437E-02],

[+1.4575962E-01,+1.3355103E-01,+1.2598168E-01,+1.1882531E-01,+1.1245899E-
01,+1.0530277E-01,+9.9349451E-02,+9.3305760E-02,+8.6987187E-02,+7.9124308E-
02,+7.0364465E-02,+5.8925228E-02,+4.8502213E-02,+3.7738231E-02,+2.8997367E-
02,+2.2558374E-02,+1.7419529E-02,+1.5036864E-02,+1.2515015E-02],

[+1.3394338E-01,+1.2313758E-01,+1.1645555E-01,+1.1036372E-01,+1.0530277E-
01,+1.2375655E-01,+9.9453555E-02,+9.4562261E-02,+8.7151744E-02,+7.8447455E-
02,+6.9426830E-02,+5.8140592E-02,+4.8070988E-02,+3.7877306E-02,+2.9504837E-
02,+2.3012359E-02,+1.7715941E-02,+1.5061397E-02,+1.2219129E-02],

[+1.2549382E-01,+1.1514362E-01,+1.0885072E-01,+1.0351414E-01,+9.9349451E-
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02,+7.1873010E-02,+6.1172664E-02,+5.1596352E-02,+4.2155666E-02,+3.4158262E-
02,+2.7668672E-02,+2.2077410E-02,+1.8895864E-02,+1.5391697E-02],

[+1.1861376E-01,+1.0878214E-01,+1.0253117E-01,+9.7197261E-02,+9.3305760E-
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02,+7.5309408E-02,+6.5400956E-02,+5.6697692E-02,+4.8167228E-02,+4.0518766E-
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02,+8.4797569E-02,+7.6342695E-02,+6.8837247E-02,+6.1585573E-02,+5.4380604E-
02,+4.7603575E-02,+4.1043694E-02,+3.6081571E-02,+3.0268036E-02],

[+9.8773297E-02,+9.2449041E-02,+8.7176116E-02,+8.2420077E-02,+7.9124308E-
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02,+9.5932433E-02,+9.1083251E-02,+8.5912764E-02,+8.0501089E-02,+7.3983506E-
02,+6.7178677E-02,+5.9944514E-02,+5.3498915E-02,+4.5703244E-02],

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02,+6.9426830E-02,+7.1873010E-02,+7.5309408E-02,+8.4797569E-02,+9.5932433E-
```

```
02,+1.0800795E-01,+1.0777174E-01,+1.0584537E-01,+1.0307407E-01,+9.7606563E-
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[+7.0830532E-02,+6.8933915E-02,+6.4852199E-02,+6.1147391E-02,+5.8925228E-
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02,+1.0777174E-01,+1.2298416E-01,+1.2690542E-01,+1.2939287E-01,+1.2645510E-
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01,+1.4846492E-01,+1.3973979E-01,+1.2720509E-01,+1.1121698E-01],

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02,+9.7606563E-02,+1.2645510E-01,+1.5290874E-01,+1.7663051E-01,+1.8878089E-
01,+1.9045242E-01,+1.8416965E-01,+1.6861073E-01,+1.4847936E-01],

[+2.7196075E-02,+2.7180976E-02,+2.5153707E-02,+2.3214689E-02,+2.2558374E-
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02,+9.0974472E-02,+1.2039518E-01,+1.4846492E-01,+1.7495438E-01,+1.9045242E-
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[+2.0282477E-02,+2.0831196E-02,+1.9418228E-02,+1.7877493E-02,+1.7419529E-
02,+1.7715941E-02,+2.2077410E-02,+2.7860870E-02,+4.1043694E-02,+5.9944514E-
02,+8.2977977E-02,+1.1180304E-01,+1.3973979E-01,+1.6700804E-01,+1.8416965E-
01,+1.9552225E-01,+1.9637976E-01,+1.8289759E-01,+1.6484417E-01],

[+1.6480811E-02,+1.7531716E-02,+1.6626404E-02,+1.5401913E-02,+1.5036864E-
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02,+7.4879065E-02,+1.0143799E-01,+1.2720509E-01,+1.5236096E-01,+1.6861073E-
01,+1.8040823E-01,+1.8289759E-01,+1.7365334E-01,+1.5951999E-01],

[+1.2681867E-02,+1.4114632E-02,+1.3696698E-02,+1.2795437E-02,+1.2515015E-
02,+1.2219129E-02,+1.5391697E-02,+1.9532473E-02,+3.0268036E-02,+4.5703244E-
02,+6.4795076E-02,+8.8351673E-02,+1.1121698E-01,+1.3359072E-01,+1.4847936E-
01,+1.6050618E-01,+1.6484417E-01,+1.5951999E-01,+1.5063304E-01]])
```

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 'COX.inp'
## normally these will be read from the Forli CO products (CO_H_EIGENVALUES and CO_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_CO import * ## Get the apriori error covariance matrix Sa

line_type=0
with open('COX.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 (CO_H_EIGENVALUES)
            line_type=1
        elif line_type==1:
            V=fromstring(line,dtype=float, sep=',') ## V (CO_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(19-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))
```

COX.inp:

```
#File format:
#
# #comment
# E(1..10)
# V(1..190)
#
# As dumped from ..... in csv format
# Missing Values are represented by NaN
#
# 19 Levels Example
1.0,1.0,1.0,NaN,NaN,NaN,NaN,NaN,NaN,NaN
3.96400600E+00,9.71308600E+00,1.31334200E+01,1.50010900E+01,1.55852200E+01,1.50846700E+01,1.40684200E+01,1.29645600E+01,1.16968200E+01,1.01377000E+01,8.41677800E+00,6.71021300E+00,5.24768800E+00,4.062
```

76300E+00,3.04421000E+00,2.18189700E+00,1.53247400E+00,1.02236500E+00,3.41380900E-01,7.89270300E-01,1.66853400E+00,1.51684100E+00,1.02546800E+00,4.80935600E-01,5.19184900E-04,-3.80105000E-01,-6.74182200E-01,-8.99606300E-01,-1.01516800E+00,-1.02769800E+00,-9.69853700E-01,-8.82844000E-01,-7.84168300E-01,-6.66500900E-01,-5.36547500E-01,-4.20216100E-01,-3.09224200E-01,-3.06734300E-01,-5.91838100E-02,-1.90331400E-01,-1.45475100E-01,-2.80174000E-02,8.53247100E-02,1.21175000E-01,1.17189800E-01,1.11908100E-01,9.67992900E-02,5.04740700E-02,-1.08608200E-02,-7.54073700E-02,-1.27489000E-01,-1.62117300E-01,-1.82365000E-01,-1.84543300E-01,-1.73223900E-01,-1.48792600E-01,-5.46247500E-01,NaN

18 Levels Example
1.0,1.0,1.0,NaN,NaN,NaN,NaN,NaN,NaN,NaN
7.44521900E+00,1.12834200E+01,1.39313200E+01,1.47923500E+01,1.43143500E+01,1.34820000E+01,1.25611600E+01,1.13231100E+01,9.78766500E+00,8.14237200E+00,6.52749800E+00,5.10763700E+00,3.89489700E+00,2.88934000E+00,2.09735600E+00,1.47121600E+00,9.68012200E-01,3.77449300E-01,1.00296100E+00,1.19666100E+00,9.72101900E-01,5.81879400E-01,1.77577700E-01,-1.68328000E-01,-4.51181700E-01,-6.69898500E-01,-7.94804400E-01,-8.37206600E-01,-8.19269000E-01,-7.64324300E-01,-6.79304300E-01,-5.80332200E-01,-4.81448700E-01,-3.81734600E-01,-2.79913300E-01,-3.35919300E-01,-1.19924900E-01,-1.68482100E-01,-7.92111200E-02,2.03331100E-02,6.66119700E-02,9.52548500E-02,1.19731700E-01,1.17910900E-01,8.02947400E-02,2.64326800E-02,-3.42889200E-02,-8.85806900E-02,-1.27818300E-01,-1.50637900E-01,-1.58102400E-01,-1.51627100E-01,-1.30971500E-01,-5.04658400E-01,NaN

COX.out:

19 Levels Example
```
S =  [[ 0.1331821   0.03083922  0.00087426 -0.0102217  -0.01333784 -0.01763526
  -0.01438627 -0.0121519  -0.00912242 -0.00525265 -0.00109281  0.0047547
   0.01110649  0.01710152  0.02029282  0.02148602  0.02146417  0.01939328
   0.01684124]
 [ 0.03083922  0.02398163  0.00831993 -0.00051167 -0.00476872 -0.00962293
  -0.00835674 -0.00777414 -0.00638904 -0.00438389 -0.00206996  0.00115539
   0.00418719  0.00671835  0.00811126  0.00884211  0.00909755  0.00842951
   0.00755641]
 [ 0.00087426  0.00831993  0.01107203  0.00476135  0.0006242  -0.0044111
  -0.00409905 -0.00463693 -0.00458682 -0.00390332 -0.00317074 -0.00182496
  -0.00060383  0.0003371   0.00114315  0.00193778  0.00252596  0.00269282
   0.00280754]
 [-0.0102217  -0.00051167  0.00476135  0.00705078  0.00521098  0.00032268
   0.00021892 -0.00131998 -0.00237597 -0.00312534 -0.00369152 -0.00401564
  -0.00425076 -0.00457678 -0.00440565 -0.00375723 -0.00305728 -0.00233406
  -0.0015156 ]
 [-0.01333784 -0.00476872  0.0006242   0.00521098  0.00760872  0.00336986
   0.00329844  0.00129443 -0.00050845 -0.0022288  -0.00367671 -0.00506454
  -0.00625389 -0.00739175 -0.00770858 -0.00725884 -0.00658947 -0.00559949
  -0.00441706]
 [-0.01763526 -0.00962293 -0.0044111   0.00032268  0.00336986  0.02422035
   0.00526035  0.00389255  0.00022528 -0.0032595  -0.00596062 -0.00818304
```

-0.00978784 -0.01106159 -0.01138576 -0.0111022 -0.01048228 -0.00940807
-0.00807077]
[-0.01438627 -0.00835674 -0.00409905 0.00021892 0.00329844 0.00526035
0.01306279 0.00732899 0.00425685 0.0001354 -0.00354314 -0.00683745
-0.0093399 -0.01117403 -0.01194253 -0.01209469 -0.01184499 -0.01091479
-0.00969425]
[-0.0121519 -0.00777414 -0.00463693 -0.00131998 0.00129443 0.00389255
0.00732899 0.01266931 0.00690284 0.00271187 -0.00175766 -0.00582571
-0.00875131 -0.01087932 -0.01199722 -0.0126196 -0.0127528 -0.01210199
-0.01109037]
[-0.00912242 -0.00638904 -0.00458682 -0.00237597 -0.00050845 0.00022528
0.00425685 0.00690284 0.01150891 0.00705177 0.00300032 -0.0022055
-0.00607859 -0.00889793 -0.01065905 -0.01187377 -0.01235411 -0.01177243
-0.01091039]
[-0.00525265 -0.00438389 -0.00390332 -0.00312534 -0.0022288 -0.0032595
0.0001354 0.00271187 0.00705177 0.01200161 0.0086239 0.00367886
-0.00065159 -0.00420441 -0.00672717 -0.00861551 -0.00958521 -0.00932132
-0.00885101]
[-0.00109281 -0.00206996 -0.00317074 -0.00369152 -0.00367671 -0.00596062
-0.00354314 -0.00175766 0.00300032 0.0086239 0.01500759 0.01088221
0.0066111 0.00275527 -0.00040017 -0.00289945 -0.00447731 -0.00459457
-0.00466839]
[0.0047547 0.00115539 -0.00182496 -0.00401564 -0.00506454 -0.00818304
-0.00683745 -0.00582571 -0.0022055 0.00367886 0.01088221 0.01798798
0.01597278 0.01402347 0.01138601 0.00840928 0.00620047 0.00503033
0.00364954]
[0.01110649 0.00418719 -0.00060383 -0.00425076 -0.00625389 -0.00978784
-0.0093399 -0.00875131 -0.00607859 -0.00065159 0.0066111 0.01597278
0.02346752 0.02475672 0.02414934 0.02181422 0.0193526 0.01696274
0.01402386]
[0.01710152 0.00671835 0.0003371 -0.00457678 -0.00739175 -0.01106159
-0.01117403 -0.01087932 -0.00889793 -0.00420441 0.00275527 0.01402347
0.02475672 0.03366672 0.03610488 0.0355627 0.0336866 0.02998541
0.02541345]
[0.02029282 0.00811126 0.00114315 -0.00440565 -0.00770858 -0.01138576
-0.01194253 -0.01199722 -0.01065905 -0.00672717 -0.00040017 0.01138601
0.02414934 0.03610488 0.04389555 0.04593435 0.04538212 0.04101789
0.03549012]
[0.02148602 0.00884211 0.00193778 -0.00375723 -0.00725884 -0.0111022
-0.01209469 -0.0126196 -0.01187377 -0.00861551 -0.00289945 0.00840928
0.02181422 0.0355627 0.04593435 0.05395582 0.05610019 0.05207677
0.0467044]
[0.02146417 0.00909755 0.00252596 -0.00305728 -0.00658947 -0.01048228
-0.01184499 -0.0127528 -0.01235411 -0.00958521 -0.00447731 0.00620047
0.0193526 0.0336866 0.04538212 0.05610019 0.06178853 0.05890056
0.05477059]
[0.01939328 0.00842951 0.00269282 -0.00233406 -0.00559949 -0.00940807
-0.01091479 -0.01210199 -0.01177243 -0.00932132 -0.00459457 0.00503033
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   1.31198731e-01   1.40657865e-01   1.39754200e-01   1.31755590e-01
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  -7.38711121e-03  -6.29300374e-03]
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