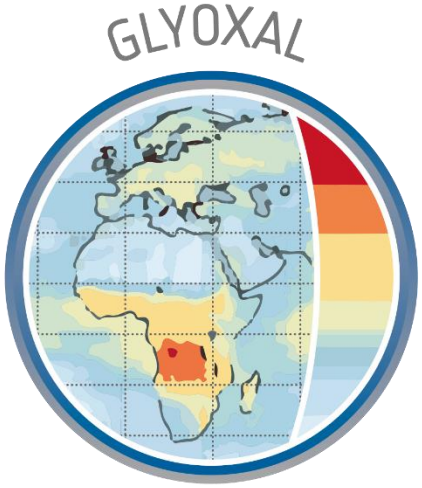
GLYoxal Retrievals from TROPOMI (GLYRETRO)

Sentinel-5p + Innovation - Theme 1: CHOCHO



Auxiliary User Manual

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Applicable Documents

[AD1] Preparing elevation data for Sentinel 5 precursor. source: KNMI, S5P-KNMI-L2-0121-TN; Issue 2.0.0, 2015-09-11.

1 Introduction

The purpose of this Auxiliary User Manual (AUM) is to provide information on which files are used in the project as input for the processor and for the verification and validation of the products. It also provides information on the format of these files in order to allow users to read and use these files.

Following this overall aim, the document is divided into three parts, describing the input files of the processor, the independent verification files and the independent validation data set.

2 Input files of the processor

The processor consists of three parts: The DOAS fit, the AMF computation and the background offset correction. The two first modules require auxiliary input data, which are described in the following sections. Additional auxiliary information are also needed for filtering purposes.

2.1 Input files for the DOAS fit

The DOAS fit needs the following input files:

1. Lv1 spectra of radiance and irradiance from the Sentinel-5 Precursor ground segment (AUX_01 and AUX_02)
2. The cross-sections of all absorbers and pseudo-absorbers used in the glyoxal fit preconvolved at the TROPOMI spectral resolution using the keydata slit functions, further optimized internally (AUX_03 – AUX_10).
3. The Fraunhofer line atlas for wavelength calibration preconvolved at the TROPOMI spectral resolution using the keydata slit functions, further optimized internally (AUX_11).
4. The slit function parameters from the Sentinel-5 Precursor keydata and further optimized internally (AUX_12). Note that those functions are not really needed as input of the processor as the cross-sections are already pre-convolved. They are nevertheless provided for traceability concerns.

While lv1 radiances and irradiances are provided in NetCDF, the other input files are in plain ASCII format.

2.2 Input files for AMF computation

The conversion of the slant columns to vertical columns requires the computation of air mass factors. This step requires a number of auxiliary data listed below:

1. A precomputed lookup table of Box-AMF (AUX_A13); this also includes AMF Jacobians needed for the calculation of error estimates.

2. Data providing the observation geometry and characterizing the scene for the extraction of the appropriate Box-AMF, i.e.
   a. Observation angles and measurement time, extracted from the L1b radiance files (AUX_01).
   b. A surface LER climatology. The current baseline is to use the monthly minimum reflectance data from the OMI climatology (AUX_14). Other options will be investigated during the project.
   c. A topography is needed. We use the GMTED2010 database (AUX_15) that has a spatial resolution up to 7.5-arc-second. Note that we actually extract dynamically the surface altitude for every observation from the operational NO2 product (AUX_17). The latter uses the same data base degraded at a coarser resolution (~10km), more representative of the TROPOMI measurements as described in [AD1]. This avoids repeating similar operations and the NO2 product is also needed for other input data (see below). Nevertheless, we also need the GMTED2010 database degraded at the resolution of the model providing a priori profiles (1°x1°) for fine scaling them according to the scene altitude.

3. The AMF computation requires to make assumptions on the vertical distribution of the glyoxal concentration in the atmosphere. Over lands, we use a priori glyoxal profile shapes provided by the CTM MAGRITTE run at BIRA-IASB (AUX_16). Over oceans, we use one single profile that has been measured in the tropical Pacific with an air-borne MAX-DOAS instrument (AUX_16).

Those different data sets are formatted in either NetCDF (GMTED2010, Box-AMF LUT, CTM profiles) or HDF5 (LER climatology). Only the single oceanic profile is formatted in plain ASCII.

2.3 Input files for auxiliary information

A series of additional input parameters are either used by the processor for selecting subset of observations or provided in the ouput L2 files for user convenience. Those additional parameters are extracted from the operational NO2 product in a dynamical way (AUX_17). Those parameters are:

1. The cloud fraction retrieved by the NO2 processor in the visible spectral range. No cloud correction is applied in the current baseline but a stringent filter is applied based on this variable.
2. The FRESCO cloud pressure and aerosol index are copied in the output files for possible post-filtering.
3. The snow/ice and surface classification flags are also extracted from the NO2 product and are respectively used for selecting appropriate pixels in the background correction and appropriate a priori profile in the AMF step (Land or Ocean pixel).

An overview on the input files can be found in Table 2-1. Static input data are also available in the password-protected data pool on the project website (https://glyretro.aeronomie.be/index.php/data). Details on the relevant variables read from the files are given from Table 2-2 to Table 2-13.

Table 2-1: Overview of auxiliary files used in the CHOCHO processor

ID	Name	Short Description	Format	Size	Static/ Dynamic	Spatial Coverage	Spatial Representation Type	Generation Frequency	Validity	Source
AUX_01	S5P_OFFL_L1B_RA_BD4_YYYYMMDDTHHMMSS_YYYYMMDDTHHMMSS_OOOOO_...nc	Band 4 lv1 radiance files from S5P	netCDF	3.7 GB	D	global	native	14 per day	N/A	DLR
AUX_02	S5P_OFFL_L1B_IR_UVN_YYYYMMDDTHHMMSS_....nc	UV/vis lv1 irradiance files from S5P	netCDF	30 MB	D	N/A	native	daily	N/A	DLR
AUX_03	AUX03_glyoxal_0.001nmFWHM_IUPbremen_400-500_S5P_OPT_SFP.xs	glyoxal cross-section preconvolved at the TROPOMI spectral resolution	ASCII	72 MB	S	N/A	N/A	N/A	N/A	Volkamer et al., 2005
AUX_04	AUX04_no2_220_cb_vac_I05e15_S5P_OPT_SFP.xs	NO_2 cross-section at 220K preconvolved at the TROPOMI spectral resolution with I0-correction	ASCII	72 MB	S	N/A	N/A	N/A	N/A	Vandaele et al., 1998
AUX_05	AUX05_NO2_296_vac_I05e15_S5P_OPT_SFP.xs	NO_2 cross-section at 296K preconvolved at the TROPOMI spectral resolution with I0-correction	ASCII	72 MB	S	N/A	N/A	N/A	N/A	Vandaele et al., 1998

AUX_06	AUX06_h2o_20180425_HITRAN2012_H2O-300-800-ground2_wc20_293K_1013hPa_S5P_OPT_SFP.xs	Water Vapor cross-section generated at 293K and 1013hPa and preconvolved at the TROPOMI spectral resolution	ASCII	72 MB	S	N/A	N/A	N/A	N/A	Rothman et al., 2013
AUX_07	AUX07_O3_223_serdyuch_poly2_I0_2e19_S5P_OPT_SFP.xs	O3 cross-section at 223K preconvolved at the TROPOMI spectral resolution with I0-correction	ASCII	72 MB	S	N/A	N/A	N/A	N/A	Serdyuchenko et al., 2014
AUX_08	AUX08_O4293_thalman_volkamer_293K_Reformat_S5P_OPT_SFP.xs	O4 cross-section at 293K preconvolved at the TROPOMI spectral resolution	ASCII	72 MB	S	N/A	N/A	N/A	N/A	Thalman and Volkamer, 2013
AUX_09	AUX09_ring_S5P_OPT_SFP.xs	Ring cross-section at the TROPOMI spectral resolution	ASCII	72 MB	S	N/A	N/A	N/A	N/A	BIRA-IASB
AUX_10	AUX10_water_Mason2016_450cols.xs	Liquid water cross-section	ASCII	1 MB	S	N/A	N/A	N/A	N/A	Mason et al., 2016
AUX_11	AUX11_sao2010_400-500.solref_S5P_OPT_SFP.xs	Fraunhofer atlas preconvolved at the TROPOMI spectral resolution	ASCII	72MB	S	N/A	N/A	N/A	N/A	Chance and Kurucz, 2010
AUX_12	AUX12_ISRFv3_OPT_band4.zip (based on	Optimized slit functions for band 4 of S5P	450 ASCII files providing reformatte	66MB	S	N/A	N/A	N/A	N/A	KNMI BIRA-IASB

	S5P_OPER_AUX_ISRF___00000101T000000_99991231T235959_20180320T084215.nc)		d keydata ISRF (one per row) + 450 ASCII files providing stretch factors of keydata ISRF							
AUX_13	AUX13_BIRA_AMF_I_ERR_CHOCHO_V1.1c.nc	Box-AMF lookup table computed with VLIDORT	NetCDF	36 MB	S	N/A	N/A	N/A	N/A	BIRA-IASB Spurr and Christi, 2019
AUX_14	AUX14_OMI-Aura_L3-OMLER_2005m01-2009m12_v003-2010m0503t063707.he5	OMI LER climatology	HDF5	310 MB	S	global	gridded	N/A	N/A	Kleipool et al., 2008
AUX_15	AUX15_GMTED2010_1_1_30arc.nc	Topography degraded at the resolution of 1°x1°	NetCDF	100 kB	S	global	gridded	N/A	N/A	BIRA-IASB Danielson and Gesch, 2011
AUX_16	AUX16_AprioriProfiles.zip	A priori glyoxal profile database for 2018	Zipped folder containing NetCDF files (one	3.5 GB	S (to be extended for future years)	global	gridded (profile)	offline	2018	BIRA-IASB Müller et al., 2018, 2019

			per month) with MAGRITTE data and one ASCII file containing the oceanic profile							Volkamer et al., 2015
AUX_17	S5P_OFFL_L2__NO2____YYYYMMDDTHHMMSS_YYYYMMDDTHHMMSS_OOOOO.nc	S5P NO2 operational product	NetCDF	300-450MB	D	global	native	14 per day	N/A	KNMI

Table 2-2: Details on the variables read from the lv1 radiance files (AUX_01)

Variable Names	Variable Description	Comments	Variable Units
BAND4_RADIANCE/STANDARD_MODE/INSTRUMENT/nominal_wavelength	wavelength in vacuum		nm
BAND4_RADIANCE/STANDARD_MODE/OBSERVATIONS/radiance	radiance		$mol.m^{-2}.nm^{-1}.sr^{-1}.s^{-1}$
BAND4_RADIANCE/STANDARD_MODE/GEODATA/solar_azimuth_angle BAND4_RADIANCE/STANDARD_MODE/GEODATA/solar_zenith_angle BAND4_RADIANCE/STANDARD_MODE/GEODATA/viewing_azimuth_angle BAND4_RADIANCE/STANDARD_MODE/GEODATA/viewing_zenith_angle BAND4_RADIANCE/STANDARD_MODE/OBSERVATIONS/delta_time BAND4_RADIANCE/STANDARD_MODE/OBSERVATIONS/scanline BAND4_RADIANCE/STANDARD_MODE/OBSERVATIONS/ground_pixel	solar and viewing geometry		deg
BAND4_RADIANCE/STANDARD_MODE/GEODATA/latitude BAND4_RADIANCE/STANDARD_MODE/GEODATA/longitude BAND4_RADIANCE/STANDARD_MODE/GEODATA/latitude_bounds BAND4_RADIANCE/STANDARD_MODE/GEODATA/longitude_bounds	geolocation information		deg
BAND4_RADIANCE/STANDARD_MODE/OBSERVATIONS/ground_pixel_quality BAND4_RADIANCE/STANDARD_MODE/OBSERVATIONS/measurement_quality BAND4_RADIANCE/STANDARD_MODE/OBSERVATIONS/spectral_channel_quality	flagging information		-

Table 2-3: Details on the variables read from the lv1 irradiance files (AUX_02)

Variable Names	Variable Description	Comments	Variable Units
BAND4_IRRADIANCE/STANDARD_MODE/INSTRUMENT/nominal_wavelength	wavelength in vacuum		nm
BAND4_IRRADIANCE/STANDARD_MODE/OBSERVATIONS/irradiance	irradiance		$mol.m^{-2}.nm^{-1}.s^{-1}$
BAND4_IRRADIANCE/STANDARD_MODE/OBSERVATIONS/measurement_quality BAND4_IRRADIANCE/STANDARD_MODE/OBSERVATIONS/spectral_channel_quality	flagging information		-

Table 2-4: Details on the variables read from the cross-section files (AUX_03 – AUX_10)

Variable Names	Variable Description	Comments	Variable Units

column 1	wavelength in vacuum		nm
column 2-451	cross-section convolved at the resolution of row #1-450		$cm^2.molec^{-1}$ (AUX_03-08) m^{-1} (AUX_10) No Unit (AUX_09)

Table 2-5: Details on the variables read from the Fraunhofer atlas file (AUX_11)

Variable Names	Variable Description	Source/Reference/Citation	Variable Units
column 1	wavelength in vacuum		nm
column 2-451	Irradiance convolved at the resolution of row #1-450		$Photons.cm^{-2}.nm^{-1}.s^{-1}$

Table 2-6: Details on the variables read from the slit function files (AUX_12) Files "band_4_row_XXX.txt"

Variable Names	Variable Description	Comments	Variable Units
row 1	reference wavelength in vacuum		nm
column 1	delta wavelength of slit function with respect to reference wavelength		nm
columns 2-89	Slit function values for reference wavelength and row XXX; reformatted from keydata ISRF file.		-

Table 2-7: Details on the variables read from the slit function files (AUX_12) Files "band_4_StretchFactors_row_XXX.txt"

Variable Names	Variable Description	Comments	Variable Units
column 1	reference wavelength in vacuum		nm
column 2	Stretch Factors to be applied to the delta wavelength grid (negative part) of the slit function for row XXX		-
column 3	Stretch Factors to be applied to the delta wavelength grid (positive part) of the slit function for row XXX		-

Table 2-8: Details on the variables read from the Box-AMF file (AUX_13)

Variable Names	Variable Description	Comments	Variable Units
bamf	Tabulated box-AMF (6 dimensions)		-
muo	solar zenith angle (1 dimension)	at surface bamf dimension variable	deg
mu	viewing zenith angle (1 dimension)	at surface bamf dimension variable	deg
phi	relative azimuth angle (1 dimension)	at surface bamf dimension variable	deg
alb	surface albedo (1 dimension)	bamf dimension variable	-
suf_h	surface height (1 dimension)	bamf dimension variable	km
suf_p	surface pressure (1 dimension)	bamf dimension variable	hPa
suf_idx	Layer index of surface level in profile grid (1 dimension)	bamf dimension variable	-
pi	pressure grid (at layer interfaces) (1 dimension)	bamf dimension variable	hPa
pm	pressure grid (at mid-layer) (1 dimension)	bamf dimension variable	hPa
zi	altitude grid (at layer interfaces) (1 dimension)	bamf dimension variable	km
zm	altitude grid (at mid-layer) (1 dimension)	bamf dimension variable	km
jacobians	AMF sensitivity table (8 dimensions)		-
muo_err	solar zenith angle (1 dimension)	at surface jacobians dimension variable	deg
mu_err	viewing zenith angle (1 dimension)	at surface jacobians dimension variable	deg
alb_err	surface albedo (1 dimension)	jacobians dimension variable	-
suf_h_err	surface height (1 dimension)	jacobians dimension variable	km
suf_p_err	surface pressure (1 dimension)	jacobians dimension variable	hPa
ph_err	profile effective height (1 dimension)	jacobians dimension variable	-
cf_err	cloud fraction (1 dimension)	jacobians dimension variable	-

cp_err	cloud_pressure (1 dimension)	jacobians dimension variable	hPa

Table 2-9: Details on the variables read from LER database (AUX_14)

Variable Names	Variable Description	Comments	Variable Units
/HDFEOS/GRIDS/EarthSurfaceReflectanceClimatology/Data Fields/MonthlyMinimumSurfaceReflectance	Reflectance (4 dimensions) at 452 nm		-
/HDFEOS/GRIDS/EarthSurfaceReflectanceClimatology/Data Fields/Latitude	Latitude grid (1 dimension)	Reflectance dimension variable	deg
/HDFEOS/GRIDS/EarthSurfaceReflectanceClimatology/Data Fields/Longitude	Longitude grid (1 dimension)	Reflectance dimension variable	deg
/HDFEOS/GRIDS/EarthSurfaceReflectanceClimatology/Data Fields/Wavelength	wavelength grid (1 dimension)	Reflectance dimension variable	nm

Table 2-10: Details on the variables read from topography (AUX_15)

Variable Names	Variable Description	Comments	Variable Units
altitude	surface altitude (2 dimensions)	degraded at resolution of 1°x1° from original GMTED2010 database	m
latitude	latitude grid (1 dimension)	altitude dimension variable	deg
longitude	longitude grid (1 dimension)	altitude dimension variable	deg

Table 2-11: Details on the variables read from the a priori profile database (AUX_16) Files "GLY_13h30_MAGRITTE_1x1_YYYYMM.nc"

Variable Names	Variable Description	Comments	Variable Units
VMR	glyoxal concentration from the CTM MAGRITTE (4 dimensions) for year YYYY and month MM	1°x1° spatial resolution 1 day time resolution	v/v
Latitude	latitude grid (1 dimension)	VMR dimension variable	deg
Longitude	longitude grid (1 dimension)	VMR dimension variable	deg

Pressure_hPa	pressure grid of the vertical concentration profile (3 dimensions)	1°x1° spatial resolution 1 month time resolution	hPa
Altitude_km	altitude grid of the vertical concentration profile (3 dimensions)	1°x1° spatial resolution 1 month time resolution	km

Table 2-12: Details on the variables read from the a priori profile database (AUX_16) File "OceanicProf4AMF_20170626.dat"

Variable Names	Variable Description	Comments	Variable Units
column 1	altitude		km
column 2	glyoxal concentration profile measured with an air-borne MAX-DOAS during the TORERO campaign in the tropical Pacific Ocean (Jan/feb 2012)	Volkamer et al., 2015	pptv

Table 2-13: Details on the variables read from the NO2 operational product (AUX_17)

Variable Names	Variable Description	Comments	Variable Units
/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS/ cloud_fraction_crb_nitrogendioxide_window	effective cloud fraction retrieved at 440 nm		-
/PRODUCT/SUPPORT_DATA/INPUT_DATA/ cloud_presure_crb	cloud optical centroid presure	not used by the processor	Pa
/PRODUCT/SUPPORT_DATA/INPUT_DATA/ surface_altitude	surface altitude	Mean of the GMTED2010 database values falling within the satellite field of view	m
/PRODUCT/SUPPORT_DATA/INPUT_DATA/ snow_ice_flag	snow ice flag		-
/PRODUCT/SUPPORT_DATA/INPUT_DATA/ surface_classification	surface classification flag	Used to discriminate lands and oceans	-
/PRODUCT/SUPPORT_DATA/INPUT_DATA/ aerosol_index_354_388	absorbing aerosol index	not used by the processor	-

3 Verification files

This section will be added in the second version of the AUM.

4 Validation files

This section will be added in the second version of the AUM.

5 References

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