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v1.1	11.2.2019	Information on IASI updated	1.1.6, 2.1.1, 2.1.3.2, 3.2.2, 4.3; References
	12.2.2019	Information on OMPS nadir mapper added (L2 to L3)	3.1.3, 4.1, 4.2
	15.2.2019	Information on limb and occultation profiles updated	1.2.9, 2.1.3.3
		Information on SMR updated	1.2.5
		Information on OMPS limb profiler updated	2.1.1
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v2.0	25.3.2021	Update	Related documents
v2.1	30.4.2021	Update after revision by ASSIMILA	All

Related documents

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Acronyms

Acronym	Definition
ACE-FTS	Atmospheric Chemistry Experiment – Fourier Transform Spectrometer
ATBD	Algorithm Theoretical Basis Document
ATSR	Along Track Scanning Radiometer
BIRA-IASB	Belgian royal Institute for Space Aeronomy
C3S	Copernicus Climate Change Service (EU)
CCI	Climate Change Initiative
CDR	Climate Data Record
CF	Climate Forecast (Conventions and Metadata)
CMA	China Meteorological Administration
CNES	Centre National d'Études Spatiales (France)
CNR	Consiglio Nazionale delle Ricerche (Italy)
CNSA	China National Space Administration
CRG	Climate Research Group
DARD	Data Access Requirements Document
DEM	Digital Elevation Model
DHF	Data Host Facility
DIAL	Differential Absorption Lidar
DLR	German Aerospace Centre
DOAS	Differential optical absorption spectroscopy
DoD	Department of Defense (USA)
DU	Dobson unit
ECMWF	European Centre for Medium-Range Weather Forecasts
ECV	Essential Climate Variable
Envisat	Environmental Satellite (ESA)
EO	Earth Observation
EOF	Empirical orthogonal function
EOS	Earth Observing System
EP	Earth Probe
ERBS	Earth Radiation Budget Satellite
ERS	European Remote-Sensing Satellite
ESA	European Space Agency
ESD	Estimated Standard Deviation
EU	European Union
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
FMI	Finnish Meteorological Institute
FOR	Field Of Regard
FORLI	Fast Optimal/Operational Retrieval on Layers for IASI

Acronym	Definition
GAW	Global Atmosphere Watch
GCOS	Global Climate Observation System
GDP	GOME Data Processor
GODFIT	GOME-type direct-fitting retrieval algorithm
GOME	Global Ozone Monitoring Experiment (aboard ERS-2)
GOME-2	Global Ozone Monitoring Experiment – 2 (aboard Metop-A)
GOMOS	Global Ozone Monitoring by Occultation of Stars
GTO	GOME-type Total Ozone
HALOE	Halogen Occultation Experiment
HARMOZ	Harmonised Level-2 ozone profiles from limb and occultation sensors
IAA	Instituto de Astrofisica de Andalucia
IAMAP	International Association of Meteorology and Atmospheric Physics
IASI	Infrared Atmospheric Sounding Interferometer
IFAC	Istituto di Fisica Applicata “Nello Carrara”
IO3C	International Ozone Commission
IMK	Institute for Meteorology and Climate Research
IPA	Independent pixel approximation
IR	Infra-Red
IRI	Infra-Red Imager
IUP	Institute of Environmental Physics, University of Bremen
ICDR	Intermediate Climate Data Record
KIT	Karlsruhe Institute of Technology
KMI-IRM	Royal Meteorological Institute of Belgium
KNMI	Royal Netherlands Meteorological Institute
LATMOS	Laboratoire Atmosphères et Observations Spatiales
LS	Low Stratosphere
LTE	Local thermodynamic equilibrium
LUT	Look-up table
Metop	Meteorological Operational Platform (EUMETSAT)
MIPAS	Michelson Interferometer for Passive Atmospheric Sounding
MLER	Minimum Lambertian Equivalent Reflectivity
MLS	Microwave Limb Sounder
MS	Multiple scattering
MSR	Multi-Sensor Reanalysis
MZM	Monthly Zonal Mean
NASA	US National Aeronautics and Space Administration
NDACC	Network for the Detection of Atmospheric Composition Change
NetCDF	Network Common Data Form (data file format)
NKUA	National and Kapodistrian University of Athens
NOAA	US National Oceanic and Atmospheric Administration
NPP	Suomi National Polar-orbiting Partnership (NOAA / NASA / DoD)

Acronym	Definition
NSMC	National Satellite Meteorological Center (China)
O_3	Ozone
OMI	Ozone Monitoring Instrument (aboard EOS-Aura)
OMPS	Ozone Mapping and Profiler Suite
OMPS-LP	OMPS Limb Profiler
OMPS-NM	OMPS Nadir Mapper
OSIRIS	Optical Spectrograph and InfraRed Imaging System (aboard Odin)
PCA	Principal component analysis
PSD	Product Specification Document
PUG	Product User Guide
RAL	Rutherford Appleton Laboratory
RMIB	Royal Meteorological Institute of Belgium
RMS	Root mean square
RT	Radiative transfer
SAA	Solar azimuth angle
SABER	Sounding of the Atmosphere using Broadband Emission Radiometry
SAGE	Stratospheric Aerosol and Gas Experiment
SBUV	Solar Backscatter Ultraviolet Radiometer
SCIAMACHY	Scanning Imaging Absorption Spectrometer for Atmospheric CHartographY (aboard Envisat)
SHADOZ	Southern Hemisphere Additional Ozonesondes programme
SMR	Sub-Millimetre Radiometer (aboard Odin)
SPARC	Stratosphere-troposphere Processes And their Role in Climate
SPARC-DI	SPARC Data Initiative
SQWG	SCIAMACHY Quality Working Group
SVD	Singular Value Decomposition
SZA	Solar Zenith Angle
TEC	Technical Expertise Centre of CNES
TIMED	Thermosphere Ionosphere Mesosphere Energetics Dynamics
TOA	Top of the atmosphere
TOMS	Total Ozone Mapping Spectrometer
TPM	ESA Third Party Mission
UARS	Upper Atmosphere Research Satellite
UiB	Universität Bremen
UNEP	United Nations Environment Programme
UPMC	Université Pierre et Marie Curie
UT	Upper Troposphere
UV	Ultraviolet
UV-Vis	Ultraviolet and visible light
VMR	Volume Mixing Ratio
VZA	Viewing Zenith Angle

Acronym	Definition
WMO	World Meteorological Organization
WOUDC	World Ozone and Ultraviolet Radiation Data Centre

Table of Contents

Scope of the document

This document is the C3S_312b_Lot2 Ozone Algorithm Theoretical Basis Document (ATBD). Its purpose is to provide a comprehensive description of all the retrieval algorithms implemented in view of generating the C3S_312b_Lot2 ozone data package delivery. This includes specifications of data characterization, error budgets, quality flags, and auxiliary information provided with the products (e.g. averaging kernels).

Most of the algorithms described here have been developed as part of the ESA Ozone Climate Change Initiative project ([RD-13] to [RD-22]). They represent the current state-of-the-art in Europe for satellite-based ozone climate data record production, in line with the “Systematic observation requirements for satellite-based products for climate” as defined by GCOS (Global Climate Observing System) in (GCOS-107 2006, https://library.wmo.int/doc_num.php?explnum_id=3813): “Product A.7: Profile and total column of ozone”.

Executive summary

The C3S_312b_Lot2 Ozone Algorithm Theoretical Basis Document contains a full description of the retrieval algorithms needed to produce level-3 (and accompanying level-2) ozone column and profile data sets from a large number of satellite sensors operated in nadir or limb geometries in spectral ranges extending from the UV to the microwave region.

The document is organized in 4 main sections, describing respectively the satellite instruments, the input and ancillary data sets needed for the processing, the retrieval algorithms and associated forward models and finally the generated output variables. Algorithms and data products are further classified in 4 main categories:

- Ozone total column retrieval from UV-nadir sensors
- Ozone total and tropospheric column retrieval from IASI
- Ozone profile retrieval from UV-nadir sensors
- Ozone profile retrieval from limb and occultation sensors

Tables

Figures

1. Instruments

Ozone can be measured by a variety of sensors and measurements techniques. In this project, we focus more particularly on ESA and ESA Third Party Mission (ESA-TPM) sensors from which three distinct lines of ozone data products are derived: total ozone, ozone profiles at low vertical resolution from nadir sensors and ozone profiles at high vertical resolution in the stratosphere and UT/LS from limb-type sensors.

1.1 Nadir-type sensors

1.1.1 ERS-2/GOME

The GOME (Global Ozone Monitoring Experiment) instrument is a 4 channel UV/Vis grating spectrometer which observed the earth's atmosphere in nadir viewing geometry. It has a moderate spectral resolution of 0.2 - 0.4 nm and a ground-pixel size of 320 x 40 km^2 (960 x 40 km^2 for the back scan). A detailed description of the instrument is given in *Burrows et al. (1999)*. GOME was launched on ERS-2 into a sun synchronous polar orbit in April 1995, and delivered data until June 2011 when the ERS-2 platform was shut down. However as a result of aging problems of the ERS-2 platform, pointing accuracy is reduced from February 2001. This affects mainly the solar measurements of GOME, decreasing the frequency of good solar irradiance measurements and thereby increasing noise in some products. Further, since June 2003, a permanent failure of the last tape recorder on ERS-2 limits GOME coverage to areas where direct downlink of data was possible. In Ozone_cci, GOME measurements are used to retrieve total columns and vertical distributions of ozone. Because of its proven stability and of its long lifetime (16 years), GOME is generally considered as the European “Gold Standard” for total ozone measurements.

1.1.2 METOP/GOME-2

The first GOME-2 instrument was launched on-board the EUMETSAT satellite Metop-A in October 2006 *(Munro et al., 2016)*. Built on a design almost identical to GOME, it covers the same spectral range as its predecessor but with an improved spatial resolution. The nominal ground-pixel size is 80 x 40 km^2 with a global coverage in almost one day (swath of 1920 km). GOME-2 continues the measurement series started with GOME, and in this project it is therefore used to retrieve total columns and vertical distributions of ozone. Data are available since January 2007 on an operational basis. A second GOME-2 instrument was launched in 2012 on the Metop-B platform, and a third one was launched in November 2018 on Metop-C.

1.1.3 AURA/OMI

The Ozone Monitoring Instrument (OMI) is a nadir viewing imaging spectrograph that measures the solar radiation backscattered by the Earth's atmosphere and surface over the entire wavelength range from 270 to 500 nm with a spectral resolution of about 0.5 nm. OMI was launched on-board the NASA satellite AURA in July 2004. In comparison to the GOME and SCIAMACHY sensors, OMI is characterized by a larger swath width of 2600 km, which enables measurements with a daily global coverage at all latitudes. The nominal OMI pixel size of 13 × 24 km^2 at nadir is also significantly smaller. The small pixel size enables OMI to look in between the clouds, which is important for retrieving tropospheric information. The light entering the telescope is also depolarised using a scrambler, which avoids polarization-related artefacts. OMI data are available since 2004 and the instrument is still operational, however in 2007 OMI started to experience the so-called row anomaly which reduces the amount of useful measurements, despite correction algorithms being implemented in the level-1 processing chain.

1.1.4 ENVISAT/SCIAMACHY

SCIAMACHY (Scanning Imaging Absorption Spectrometer for Atmospheric CHartographY) is a multi-channel UV-Vis-NIR spectrometer launched on the ENVISAT platform in 2002. Its primary mission objective was the global monitoring of trace gases in the troposphere and in the stratosphere *(Bovensmann et al., 1999)*. The solar radiation transmitted, backscattered and reflected from the atmosphere is recorded at medium resolution (0.2 nm to 1.5 nm) over the range 240 nm to 1700 nm, and in selected regions between 2.0 µm and 2.4 µm. SCIAMACHY is particular since it has three different viewing geometries: nadir, limb, and sun/moon occultation, which yield total column values as well as distribution profiles in the stratosphere and upper troposphere. In this project both nadir and limb measurements are used in Channels 1, 2 and 3. In nadir view, used for ozone total column and vertical profile retrievals, the ground pixel size for channels 2-3 is 30x60 km^2, i.e. a resolution intermediate between GOME and OMI. The swath width of SCIAMACHY at nadir is similar to GOME (960 km), however due to the alternate nadir and limb mode operation, global coverage is only obtained in approximately 6 days. In limb view, ozone number density profiles are derived in the stratosphere by exploiting the Hartley and Chappuis spectral absorption bands in channels 1 and 3. SCIAMACHY data are available from July 2002 till April 2012 when communication with ENVISAT was lost.

1.1.5 Suomi NPP/OMPS-NM

The Ozone Mapping and Profiler Suite, aboard the Suomi-NPP platform launched in 2011, has three different instruments: two nadir modules and the limb module. The Nadir mapper (NM) aims at measuring total ozone columns and relies on 2-D CCD like OMI. With a swath width of 2800 km separated into 36 cross-track footprints, it provides daily global coverage with a spatial resolution of 50 x 50 km^2 in the nominal operations. It records backscattered radiances in the range 300-380 nm with a coarse spectral resolution of about 1.0 nm. More details on the instrument can be found in *Seftor et al. (2014)*.

1.1.6 METOP/IASI

The Infrared Atmospheric Sounding Interferometer (IASI) is a nadir looking Fourier Transform Spectrometer associated with an imaging instrument launched on the Metop series of European meteorological EUMETSAT's polar-orbit satellites. The mission is dedicated to high-resolution atmospheric sounding of trace gases like ozone, methane or carbon monoxide on a global scale and to operational meteorological soundings with a high accuracy requirement (1 K for tropospheric temperature and 10% for humidity with a vertical resolution of 1 km). Three IASI instruments have been successively launched in October 2006, in September 2012 and in November 2018 on Metop-A, -B and –C respectively. The Metop satellites are sun-synchronous with a 98.7° inclination to the equator, and a global coverage twice daily at about 09:30 and 21:30 local time. Each of the three launched Metop platforms makes a little more than 14 orbits a day. IASI is a cross-track scanner covering the infrared spectral domain from 645 to 2,760 cm^{-1} (3.62–15.5 µm) with a total of 30 ground fields of regard (FOR) per scan. The spectrum is measured in three wavelength bands (8.26–

15.5, 5.0–8.26, and 3.62–5.0 µm), with a separate detector allowing the continuous spectral coverage with no gaps, and each FOR measures a 2×2 array of footprints characterized by a 12-km diameter at nadir. The apodized spectral resolution is 0.5 cm^{-1} and each spectrum is sampled every 0.25 cm^{-1} providing a total of 8461 radiance channels.

1.1.7 BUV

The Backscatter UltraViolet experiment (BUV) onboard the Nimbus 4 satellite was the first satellite measuring ozone. It operated from April 1970 till May 1977 but with several big gaps in time without observations. The instrument measured the earth spectrum in several small bands between 252 and 340 nm. From this the total ozone and an ozone profile is derived.

1.1.8 SBUV

The Solar Backscatter Ultraviolet Radiometer, or SBUV, is a series of operational instruments on NOAA weather satellites in Sun-synchronous orbits. This instrument has flown on the Nimbus-7, NOAA-9, NOAA-11, NOAA-14, NOAA-16, NOAA-17, NOAA-18, and NOAA-19 in the period from November 1978 to Dec 2011. The instrument is very similar to its predecessor BUV.

1.1.9 TOMS

The Total Ozone Mapping Spectrometer (TOMS) is a NASA satellite instrument for measuring ozone values. Of the four TOMS instruments which were successfully launched only two are used because of the length of time period of observations: TOMS on Nimbus-7 and on EarthProbe. This covers the time periods from November 1978 to May 1993 and July 1996 to December 2002. Besides ozone a few other gases can be derived from TOMS observations.

1.1.10 FY 3/TOU

The Feng-Yun-3 (FY-3) series of satellites are a program of CMA/NSMC (China Meteorological Administration/National Satellite Meteorological Center) and CNSA (China National Space Administration). Each FY-3 satellite has a slightly different payload of various instruments. The FY 3A, 3B and 3C have a Total Ozone Unit (TOU) instrument aboard, capable of measuring total ozone. The first satellite, FY-3A, was launched on May 27, 2008.

1.2 Limb and occultation type sensors

1.2.1 ENVISAT/MIPAS

MIPAS (Michelson Interferometer for Passive Atmospheric Sounding) is an infrared limb emission sounder on ENVISAT, designed and operated for measurements of constituents between the upper troposphere and the mesosphere. MIPAS is a rear looking instrument with the lines of sight approximately in the orbit plane. In the original measurement mode, which was operational from July 2002 to March 2004, 17 tangent altitudes between 6 and 68 km were measured per limb scan at a spectral resolution of 0.035 cm^{-1} (unapodized). However from January 2005, due to a mirror failure, MIPAS operated in reduced spectral resolution mode (0.0625 cm^{-1}). MIPAS measured ozone vertical profiles day and night on the altitude range from 6 to 70 km, pole-to-pole. Data are available for July 2002-March 2004 and January 2005 until April 2012 when communication with ENVISAT was lost. Global coverage was obtained in approximately 3 days.

1.2.2 ENVISAT/GOMOS

GOMOS (Global Ozone Monitoring by Occultation of Stars) is a medium resolution spectrometer covering the wavelength range from 250 nm to 950 nm. It measures attenuation of stellar light in occultation geometry. From dark-limb occultations in the UV-Visible and IR spectral ranges, the vertical profiles of ozone are retrieved in the altitude region from 15 to 100 km. In comparison to other limb-type sensors on ENVISAT, GOMOS features a high vertical resolution of the retrieved ozone profiles: 2 km below 30 km, 3 km above 40 km, with a linear growth from 2 km to 3 km in the altitude range 30-40 km. However the quality of the retrieved profiles can depend on the type of star used as a source. Careful selection and error characterization are necessary to make best use of the data products. GOMOS data are available from 2002 till 2012. Summer poles are not covered, due to the absence of night-time conditions. Data from May-June 2003, January-July 2005 and February-November 2009 are not available due to the instrument technical anomalies.

1.2.3 ENVISAT/SCIAMACHY

See Section 1.1.4.

1.2.4 ODIN/OSIRIS

OSIRIS (Optical Spectrograph and InfraRed Imaging System) is a Canadian instrument on board the Swedish satellite Odin that was launched in February of 2001. It is a limb-viewing device that makes repeated measurements of the limb scattered radiance with a sampling of approximately 2 km between 10 km and 100 km of altitude. OSIRIS uses limb radiance spectra to generate ozone profiles in a range from 80° S to 80° N. Concentrations are retrieved on a 1 km grid from 10.5 km to 59.5 km and have the vertical resolution ~2 km. The ozone retrieval by University of Saskatchewan using a multiplicative algebraic reconstruction technique is described in *(Degenstein et al., 2009)*. The OSIRIS instrument is still operational.

1.2.5 ODIN/SMR

The Sub-Millimetre Radiometer (SMR) onboard the Odin satellite, was launched in February 2001. Measurements of thermal emission lines are performed during day and night and global coverage is achieved during one observation day. Vertical profiles of ozone and many other species are retrieved using retrieval algorithms based on the Optimal Estimation Method. The official operational level-2 data are produced by the Chalmers University of Technology in Göteborg, Sweden. In this project, we use the currently recommended version 2.1 ozone data product that provides stratospheric ozone data in the ~12-50km range with 2.5-3.5km vertical resolution and single-profile precision of about 20%. The Odin data set is available from November 2001 until present. The validation activity performed in the framework of the Ozone_cci project identified corrupted data after 2010. The reprocessing of the whole SMR mission is ongoing.

1.2.6 SCISAT/ACE-FTS

ACE-FTS is on-board the Canadian satellite SCISAT launched in August 2003, and data is available from Feb. 2004 to present. It provides latitudinal coverage from about 85°N to 85°S with complete coverage every 3 months. The ACE-FTS is a high-resolution (0.02 cm^{-1}) Fourier transform spectrometer measuring from 2.2 to 13 µm (750 – 4400 cm^{-1}). Operating in solar occultation mode, the ACE-FTS provides detailed profiles of the Earth's atmosphere for more than 30 chemical species.

The altitude range of the retrieved ozone profiles is from cloud tops (~5 km) to 95 km and the vertical resolution is ~3-4 km (based on the field-of-view of the ACE-FTS instrument).

1.2.7 ERBS/SAGE2

The SAGE II (Stratospheric Aerosol and Gas Experiment) operated in 1984-2005 on board the Earth Radiation Budget Satellite (ERBS) into a 57° inclination. It exploits the atmospheric species by using the solar occultation technique at sunrise and sunset geometries by measuring the attenuated sun light. The wavelengths used are ranging from 385 to 1200 nm in 7 channels. The 'onion-peeling' method *(Chu et al., 1989)* is used in order to invert the measured spectrum into aerosol extinction, ozone, nitrogen dioxide, and water vapor with a vertical resolution of 1 km. In this work, the version V7 of SAGE II is used *(Damadeo et al., 2013)*. Ozone is inferred from spectral measurements near 600 nm, at the peak of the Chappuis band. SAGE II provides high-quality ozone profiles with a random uncertainty < 1% in the stratosphere.

1.2.8 UARS/HALOE

Halogen Occultation Experiment (HALOE) on board the Upper Atmosphere Research Satellite (UARS) operated in 1991-2005 and provided profiles of middle atmosphere composition, temperature and aerosol extinction. HALOE is a solar occultation instrument which used thermal infrared bands *(Russel III et al., 1993)*. About 30 measurements daily split between sunrise and sunset were performed daily, and near global coverage achieved within about one and a half month. The ozone concentrations retrieved have vertical resolution of 1.6 km in the altitude range 15 -90 km.

1.2.9 TIMED/SABER

The Sounding of the Atmosphere using Broadband Emission Radiometry (SABER) instrument is one of four instruments on NASA's TIMED (Thermosphere Ionosphere Mesosphere Energetics Dynamics) satellite. The primary goal of the SABER experiment is to provide the data needed to advance our understanding of the fundamental processes governing the energetics, chemistry, dynamics, and transport in the mesosphere and lower thermosphere. SABER accomplishes this with global measurements of the atmosphere using a 10-channel broadband limb-scanning infrared radiometer covering the spectral range from 1.27 µm to 17 µm. These measurements are used to provide vertical profiles of kinetic temperature, pressure, geopotential height, volume mixing ratios for the trace species O_3, CO_2, H_2O, [O], and [H], volume emission rates for 5.3 µm NO, 2.1 µm OH, 1.6 µm OH, and 1.27 µm O2(1Δ), cooling and heating rates for many CO_2, O_3, and O_2 bands, and chemical heating rates for 7 important reactions. This study uses the SABER V2.0 ozone profiles.

1.2.10 AURA/MLS

MLS (Microwave Limb Sounder) is one of the instruments on board the Aura satellite. It was launched in 2004. It collects data with 13 orbits per day and is flying at 705 km altitude on a near polar orbit. It measures the thermal microwave emission from Earth's atmosphere and retrieves different species along with pressure, cloud ice density, and temperature *(Waters et al. 2006; Livesey, Snyder and Wagner 2006)*. MLS measures continuously the thermal emission from broad band spectra at 118, 190, 240, 640, and 2500 GHz using limb viewing geometry. The vertical resolution is 2.5 km in the stratosphere and degrades to 4 - 6 km in the mesosphere and to 3 km at 316 hPa. Supplementary information regarding screening flags, the quality of fitted spectra, and retrieval status are included along the Level 2 data sets *(Froidevaux et al., 2008)*. The retrieved MLS ozone profiles V 4.2 are used in this study.

1.2.11 SUOMI NPP/OMPS-LP

The Ozone Mapping and Profiler Suite Limb Profiler (OMPS-LP) on board the Suomi-NPP satellite has been taking measurements of limb-scattered sunlight from early 2012 to present *(Flynn et al., 2006*). OMPS-LP images the atmosphere using three vertical slits, one aligned with the orbital plane and the others separated by 250 km at the tangent point on either side of the orbital track. Imaging allows OMPS-LP to obtain along track and vertical sampling of approximately 125 km and 1 km respectively. Spectral information in the range 270—1000 nm is obtained employing a prism spectrometer.

For our analyses, the OMPS-LP ozone data processed in the University of Saskatchewan, USask 2D v1.1.0, are used (*Zawada et al., 2017*). The USask 2D retrieval accounts for atmospheric variations along the orbital track by using the SASKTRAN-HR forward model (*Zawada et al., 2015*) and simultaneously retrieving the ozone field for an entire orbit, rather than processing each vertical image separately. Only data from the center slit of OMPS is used as the other two slits are not aligned with the orbital track. Profiles are retrieved with a vertical resolution of 1–2 km and an along track resolution of 300–400 km. Individual profiles have a mean uncertainty of 4–6% for most of the upper and middle stratosphere, with values increasing to approximately 30% just below the tropopause.

2. Input and auxiliary data

2.1 Input data sets from satellites

2.1.1 Overview

Table 1 gives an overview of the satellite data needed for the generation of the C3S Ozone ECV Data products.

Table 1. Overview of satellite data required to generate the C3S ozone ECV products.

Agency	Satellite	Sensor	Period	Product	Version	Subset or complete needed	Volume	Available from	Comments
CMA/ CNSA	FY-3A	TOU	2008-2014	Level 2	V2.0.0	Complete	45 Gb	NSMC	At KNMI
CMA/CNSA	FY-3B	TOU	2010-2018	Level 2	V2.0.0	Complete	56 Gb	NSMC	At KNMI
CSA	Scisat	ACE-FTS	2004-2016	Level 2	V3.5/3.6	Complete	1 GB	ESA	On ftp server and available on Ozone_cci server
ESA	ERS-2	GOME	1995-2011	Level 1b	V4	Complete	1 TB	ESA	On D-PAF ftp server
ESA	Envisat	SCIAMACHY	2002-2012	Level 1	V7.04			ESA	
ESA	Envisat	SCIAMACHY	2002-2012	Level 1b	V8.01	Complete	16 TB	ESA	Current version v8 available now from ftp server D-MM-PAC
ESA	Envisat	SCIAMACHY	2002-2012	Level 2	V3.5	Complete	6.6 Gb	UBr	
ESA	Envisat	SCIAMACHY	2002-2012	Level 2	V5.04			ESA	
ESA	Envisat	GOMOS	2002-2012	Level 2	ALGOM2s	Complete	400 MB	ESA & FMI	On ESA/ALGOM and Ozone_cci ftp server
ESA	Envisat	MIPAS	2002-2012	Level 2	V7	Complete	6 GB	KIT/IMK	On ftp server
EUMETSAT	Metop-A	GOME-2	2006-2016	Level 1b	V4	Complete	50 TB	EUMETSAT	On media and on ftp server
EUMETSAT	Metop-B	GOME-2	2012-2016	Level 1b	V4	Complete	20 TB	EUMETSAT	On media and on ftp server
EUMETSAT	Metop-A	IASI	2008-present	Level 2	V1	Complete	7.7 TB	AERIS	On AERIS and Ozone_cci server
EUMETSAT	Metop-B	IASI	2013-present	Level 2	V1	Complete	3.3TB	AERIS	On AERIS and Ozone_cci server
NASA	Nimbus4	BUV	1970-1977	Level 2	V8.6	Complete	3 GB	NOAA/NASA	On ftp server
NASA	Nimbus7/ Earthprobe	TOMS	1978-2002	Level 2	V8	Complete	300 GB	NASA	On ftp server
NASA	Nimbus-7/ NOAA-9-19	SBUV	1978-2011	Level 2	V8.6	Complete	100 GB	NOAA/NASA	On ftp server
NASA	ERBS	SAGE-2	1984-2005	Level 2	V7	Complete	330 Mb	NASA	
NASA	UARS	HALOE	1991-2005	Level 2	V19	Complete	210 Mb	NASA	
NASA	TIMED	SABER	2002-	Level 2	V2.0	Complete	18 Gb	NASA	
NASA	AURA	OMI	2004-2016	Level 1b	V3	Complete	20 TB	NASA	On ftp server
NASA	AURA	OMI	2004-2016	OMITO3 Level 2	V3	Complete	2 TB	NASA	On ftp server
NASA	AURA	OMI	2004-2016	OMIDOAO3 Level 2	V3	Complete	2 TB	NASA	On ftp server
NASA	AURA	MLS	2004-	Level 2	V4.2	Complete	33 Gb	NASA	
NASA	Suomi-NPP	OMPS-NM	2012-	Level1b	V2.0	Complete	3 TB	NASA	On ftp server
NASA	Suomi-NPP	OMPS-LP	2012-	Level 2	V1.1.0	Complete	9 GB	USask/ESA	On ftp server (Univ. Saskatchewan) and Ozone_cci server
SNSB CSA -TPM	ODIN	SMR	2001-2016	Level 2	V2.1	Complete	15 GB	ESA / Chalmers	On ftp server (Univ. Chalmers) and Ozone_cci server
SNSB CSA -TPM	ODIN	OSIRIS	2001-2016	Level 2	V5.10	Complete	15 TB	ESA	On ftp server (Univ. Saskatchewan) and Ozone_cci server

2.1.2 Level-1 data

Level-1 data are required from the following sensors to generate total column and vertical ozone profiles. They serve as input for the level-2 retrieval algorithms that are applied in the project for the generation of the nadir ozone ECV data products.

- ERS-2 / GOME (Table 2, Table 3)
- Envisat / SCIAMACHY (Table 4, Table 5)
- Metop-A and Metop-B / GOME-2 (Table 6)
- EOS-Aura / OMI (Table 7)
- Suomi-NPP / OMPS-NM (Table 8)

Table 2. ERS-2/GOME L-1b data required as input to the C3S Ozone data processing.

Originating system	GOME flew on-board the ESA satellite ERS-2 which was launched in April 1995 and operated until September 2011. The GOME level-1b data product were generated from the ESA level 0 product at DLR.
Data class	Earth Observation Data
Sensor type and key technical characteristics	The GOME (Global Ozone Monitoring Experiment) instrument is a 4 channel UV/Vis grating spectrometer observing the earth's atmosphere in nadir viewing geometry. It has a moderate spectral resolution of 0.2 - 0.4 nm and a ground-pixel size of 320 x 40 km^2 (960 x 40 km^2 for the back scan). GOME was launched on ERS-2 into a sun synchronous polar orbit in April 1995, and delivered data until September 2011. In this project GOME measurements in Channels 1 and 2 will be used to retrieve total and vertical distribution of ozone. The wavelength range and spectral resolution of the four GOME channels are provided in Table 3.
Data availability & coverage	GOME data are available from April 1995 until September 2011 when the instrument was switched off. However as a result of aging problems of the ERS-2 platform, pointing accuracy has been reduced since February 2001. This affects mainly the solar measurements of GOME, decreasing the frequency of good solar irradiance measurements and thereby increasing noise in some products. Further, since June 2003, a permanent failure of the last tape recorder on ERS-2 has limited GOME coverage to areas where direct downlink of data was possible. With the nominal swath of 960 km, global coverage was achieved every three days at the equator and earlier at higher latitudes.
Source data product name and reference to product technical specification documents	ERS-2 GOME level 1b data *[RD-3]*.
Data quantity	Approximately 70 Gb/year (until 2003). Total volume is about 1 TB.
Data quality and reliability	The data quality is monitored as part of the operational off-line ground segment of GOME at DLR (http://atmos.caf.dlr.de/gome). For details about the quality of the GOME level-1 products we refer to the disclaimer document.
Ordering and delivery mechanism	These ESA standard GOME products are generated at DLR on behalf of ESA and are freely available. After registering at ESA EO help and Order Desk, level 1 data can be copied free-of-charge from a FTP Server.
Access conditions & pricing	The team has default access to the GOME Level-1 data. The GOME level-1 products are free of charge.

Issues	GOME level 1 version 5 using the latest calibration corrections valid for the complete GOME mission are needed. Note that the current GOME level 1 version 4 products only contain a subset of the data acquired after the ERS-2 recorder problem in 2003. A revised version is under development and will be available for processing of CCI Phase-2 products.

Table 3. Wavelength range and spectral resolution of the four GOME channels.

Channel	Wavelength range (nm)	Spectral resolution (nm)
1A	237-283	0.20
1B	283-316	0.20
2	311-405	0.17
3	405-611	0.29
4	595-793	0.33

Table 4. Envisat/SCIAMACHY L-1b data required as input to the C3S Ozone data processing.

Originating system	SCIAMACHY operated on-board the ESA satellite ENVISAT from March 2002 until April 2012. The SCIAMACHY level-1b data product is generated from the level 0 product by ESA and DLR.
Data class	Earth Observation Data
Sensor type and key technical characteristics	SCIAMACHY (Scanning Imaging Absorption Spectrometer for Atmospheric CHartographY) is an imaging spectrometer whose primary mission objective was the global monitoring of trace gases in the troposphere and in the stratosphere. The solar radiation transmitted, backscattered and reflected from the atmosphere is recorded at medium resolution (0.2 nm to 1.5 nm) over the range 240 nm to 1700 nm, and in selected regions between 2.0 µm and 2.4 µm. SCIAMACHY has three different viewing geometries: nadir, limb, and sun/moon occultation, which yield total column values as well as distribution profiles in the stratosphere and upper troposphere. In this project both nadir and limb measurements will be used in Channels 1 to 3. The ground pixel size for channels 2-3 is 30x60 km^2 (nadir view). The wavelength range and spectral resolution of the eight SCIAMACHY channels are provided in Table 5.
Data availability & coverage	SCIAMACHY data are available since 2002 and the instrument operation ended by April 2012, when the communication with ENVISAT was lost. Global coverage is obtained in approximately 6 days.
Source data product name and reference to product technical specification documents	SCIAMACHY level 1b data *[RD-8].*
Data quantity	1.95 TB / year. Total volume is about 20 TB.

Data quality and reliability	The data quality was monitored by ESA and results were reported in SCIAMACHY bimonthly report documents that described the status and changes to the SCIAMACHY instrument, its data processing chain and its data products. It was the result of input received from the different groups working on SCIAMACHY operation, calibration, product validation, and data quality. The groups contributing to the report were SOST-DLR and SOST-IFE, ESA-ESRIN PCF, ESA-ESTEC PLSO and DLR-IMF. The geophysical quality monitoring was under responsibility of the SQWG and the SCIAVALIG groups. Other monitoring services are summarized at http://www.sciamachy.org/.
Ordering and delivery mechanism	SCIAMACHY level-1 data are available from ESA and are free of charge for the team.
Access conditions & pricing	The team has default access to the SCIAMACHY Level-1 data. The SCIAMACHY level-1 products are free of charge.
Issues	The SCIAMACHY level-1 version 8 (or higher) data set including the most advanced degradation corrections is required.

Table 5. Wavelength range and spectral resolution of the eight SCIAMACHY channels.

Channel	Wavelength range (nm)	Resolution (nm)
1	240(214) – 314	0.24
2	309 – 405	0.26
3	394 – 620	0.44
4	604 – 805	0.48
5	785 – 1050	0.54
6	1000 – 1750	1.48
7	1940 – 2040	0.22
8	2265 – 2380	0.26

Table 6. Metop/GOME-2 L-1b data required as input to the C3S Ozone data processing.

Originating system	GOME-2 is on-board the EUMETSAT satellite Metop-A which was launched in October 2006. A second GOME-2 instrument was launched in September 2012 on the Metop-B platform and a third one on Metop-C in November 2018. The GOME-2 level-1b data product is generated from the level 0 product by EUMETSAT. Metop-C data are not included in the C3S ozone products.
Data class	Earth Observation Data
Sensor type and key technical characteristics	The GOME-2 instrument covers the same spectral range as GOME with an improved spatial resolution. When operated in full swath, the nominal ground-pixel size is 80 x 40 km^2 with a global coverage in almost one day (swath of 1920 km). After the launch of Metop-B, it has been decided to operate the two instruments in tandem, GOME-2B in full-swath mode and GOME-2A in reduced swath (960 km) mode. In this configuration, the nominal ground-pixel size of GOME-2A is 40 x 40 km^2. When combining the two instruments, full earth coverage is obtained in one day. In this project GOME-2 measurements in Channels 1 and 2 are used to retrieve total and vertical distribution of ozone.

Data availability & coverage	GOME-2A data are available since January 2007 on an operational basis. Likewise GOME-2B data are operationally available since July 2013. Global coverage is obtained in around 1.5 days (in 1 day when GOME-2A and GOME2-B are combined) at the equator and daily on higher latitudes.
Source data product name and reference to product technical specification documents	GOME-2 level 1b data *[RD-5].*
Data quantity	4 TB/ year. Total volume is about 36 TB until September 2014.
Data quality and reliability	The data quality is monitored by EUMETSAT and results are reported in Newsletters. Both GOME-2A and GOME-2B suffer from time-dependent degradation especially in the UV region.
Ordering and delivery mechanism	GOME-2 level-1 data are available from EUMETSAT and are free of charge for the team.
Access conditions & pricing	The team has default access to the GOME-2 A/B Level-1 data. The GOME-2 level-1 products are free of charge.
Issues	The GOME-2 level-1b version 5 data set is required.

Table 7. Aura/OMI L-1b data required as input to the C3S Ozone data processing.

Originating system	OMI is on-board the NASA satellite AURA which was launched in July 2004. The OMI level-1b data product is generated from the KNMI/NASA level 0 product at NASA.
Data class	Earth Observation Data
Sensor type and key technical characteristics	The OMI instrument is a nadir viewing imaging spectrograph that measures the solar radiation backscattered by the Earth's atmosphere and surface over the entire wavelength range from 270 to 500 nm with a spectral resolution of about 0.5 nm. The 114° viewing angle of the telescope corresponds to a 2600 km wide swath on the surface, which enables measurements with a daily global coverage. The light entering the telescope is depolarised using a scrambler and then split into two channels: the UV channel (wavelength range 270 - 380 nm) and the VIS channel (wavelength range 350 - 500 nm). In the normal global operation mode, the OMI pixel size is 13 km× 24 km at nadir (along x across track). In the zoom mode the spatial resolution can be reduced to 13 km × 12 km. The small pixel size enables OMI to look in between the clouds, which is very important for retrieving tropospheric information.
Data availability & coverage	OMI data are available since 2004 and the instrument is still operational. OMI has a daily global coverage except when operated in zoom-in mode. In 2007 OMI started to experience the so-called row anomaly. Two rows seemed to be (partially) blocked. This row anomaly was followed by other row anomalies in 2008, 2009 and 2011. Like the first row anomaly a few rows seemed to be (partially) blocked. But these rows also suffered from reflected sunlight during part of the orbit and earthshine from another scene. These new row anomalies are changing through time. Currently, progress has been made with a correction algorithm for these rows.
Source data product name and reference to product technical specification documents	Version 003 OMI Level 1B Products *[RD-6].* Orbital Swath Pixels (UV1, 13x48 km^2; UV2 & VIS, 13x24 km^2; Zoom, 13x12 km^2).
Data quantity	Approximately 1 TB/year. Total volume is about 12 TB (until September 2014).

Data quality and reliability	The quality flags "PixelQualityFlags", "GroundPixelQualityFlags", "XTrackQualityFlags", and "MeasurementQualityFlags" are available in the data for all possible errors/warning *[RD-6]*.
Ordering and delivery mechanism	The data is available via the browsable web-interface Mirador of NASA.
Access conditions & pricing	The OMI level-1 products are free of charge.
Issues	None.

Table 8. Suomi-NPP/OMPS-NM L-1b data required as input to the C3S Ozone data processing.

Originating system	OMPS-NM is on-board the NASA satellite Suomi-NPP which was launched in end of 2011. The level-1b data product v2.0 is generated from the NASA level 0 product at NASA.
Data class	Earth Observation Data
Sensor type and key technical characteristics	The Ozone Mapping and Profiler Suite, aboard the Suomi-NPP platform launched in 2011, has three different instruments: two nadir modules and the limb module. The Nadir mapper (NM) aims at measuring total ozone columns and relies on 2-D CCD like OMI. With a swath width of 2800 km separated into 36 cross-track footprints, it provides daily global coverage with a spatial resolution of 50 x 50 km^2 in the nominal operations. It records backscattered radiances in the range 300-380 nm with a coarse spectral resolution of about 1.0 nm. More details on the instrument can be found in *Seftor et al. (2014)*.
Data availability & coverage	OMPS data are available since 2012 and the instrument is still operational. OMPS has a daily global coverage except when operated in zoom-in mode.
Source data product name and reference to product technical specification documents	Version 2.0 OMPS Level 1B Products [Nadir Mapper L1B user documentation at https://ozoneaq.gsfc.nasa.gov/media/docs/NMEV-L1B_Release_Notes.pdf]
Data quantity	Approximately 0.5 TB/year. Total volume is about 4 TB (until Dec 2018).
Data quality and reliability	Data quality monitoring is under the responsibility of NASA.
Ordering and delivery mechanism	The data is available via the browsable web-interface NASA https://disc.gsfc.nasa.gov/datasets/OMPS_NPP_NMEV_L1B_V2/summary?keywords=OMPS
Access conditions & pricing	The OMPS level-1 products are free of charge.
Issues	None.

2.1.3 Level-2 data

This section is dedicated to Level-2 data that serve as input to C3S ozone data processing chains and that are not produced within the C3S Ozone project.

2.1.3.1 Ozone total column data required by the multi-sensor reanalysis (MSR)

The latest total ozone retrievals of 18 satellite instruments are used: BUV-Nimbus4, TOMS-Nimbus7, TOMS-EP, SBUV-7, -9, -11, -14, -16, -17, -18, -19, GOME, SCIAMACHY, OMI, GOME-2, FY-3A, FY-3B and OMPS.

Table 9. The satellite datasets used in the MSR. The columns show (1) the name of the dataset, (2) the satellite instrument, (3) the satellite, (4 and 5) the time period.

Data set	Instrument	Satellite	From	To
BUV	BUV	Nimbus-4	1 April 1970	6 May 1977
TOMS-N7	TOMS	Nimbus-7	31 Oct. 1978	6 May 1993
TOMS-EP	TOMS	Earth probe	25 July 1996	31 Dec. 2002
SBUVN07	SBUV	Nimbus-7	31 Oct. 1978	21 June 1990
SBUVN09	SBUV/2	NOAA-9	2 Febr. 1985	19 Febr. 1998
SBUVN11	SBUV/2	NOAA-11	1 Dec. 1988	27 Mar. 2001
SBUVN14	SBUV/2	NOAA-14	5 Febr. 1995	28 Sep.2006
SBUVN16	SBUV/2	NOAA-16	3 Oct. 2000	31 Dec. 2003
SBUVN17	SBUV/2	NOAA-17	11 July 2002	31 Dec. 2011
SBUVN18	SBUV/2	NOAA-18	5 June 2005	31 Dec. 2011
SBUVN19	SBUV/2	NOAA-19	23 Febr. 2009	31 Dec. 2011
GDP5	GOME-1	ERS-2	27 June 1995	3 July 2011
TOGOMI2	GOME-1	ERS-2	27 June 1995	3 July 2011
SGP5	SCIAMACHY	Envisat	2 Aug. 2002	8 Apr. 2012
TOSOMI2	SCIAMACHY	Envisat	2 Aug. 2002	8 Apr. 2012
OMDOAO3	OMI	Aura	1 Oct. 2004	31 Dec. 2015
OMTO3	OMI	Aura	1 Oct. 2004	31 Dec. 2015
GOME2A	GOME-2	Metop-A	4 Jan. 2007	31 Dec. 2015
OMPS	OMPS	Suomi-NPP	7 Nov. 2011	31 Dec. 2015
TOU	TOU	FY3-A	1 July 2008	13 May 2014
TOU	TOU	FY3-B	1 October 2010	30 April 2018

2.1.3.2 Ozone column data from IASI

The IASI/Metop-A and IASI/Metop-B Level 2 data required for creation of the gridded nadir ozone column data set are described in Table 10.

Table 10. Metop/IASI L-2 data required as input to the generation of C3S ozone products.

Originating system	IASI is on-board the EUMETSAT satellite Metop-A which was launched in October 2006. A second IASI instrument was launched in September 2012 on the Metop-B platform. The IASI level-2 data products are generated by applying the FORLI v20151001 radiative transfer model and retrieval algorithm to level 1C radiances to retrieve the ozone nadir vertical profile.
Data class	Earth Observation Data
Sensor type and key technical characteristics	see Section 1.1.6
Data availability & coverage	IASI/Metop-A data are available from January 2008 until present. IASI/Metop-B data are available from April 25 2013 until present.
Data quantity	Approximately 1 Gb / year. Total volume is about 11 TB.
Data quality and reliability	Total ozone: positive bias of 1-2% compared to UV observations Tropospheric ozone: negative bias of ~10% compared to ozone sondes *Boynard et al. (2016, 2018)*
Ordering and delivery mechanism	The data are available from the AERIS (2008-present) and O3-CCI (2008-2016) website

2.1.3.3 Limb and occultation ozone profile data

The following Level 2 data are required for creation of Level 3 data and the merged limb ozone profile data set.

- Envisat / GOMOS (Table 11)
- Envisat / MIPAS (Table 12)
- Envisat / SCIAMACHY (Table 13)
- Odin / OSIRIS (Table 14)
- Odin / SMR
- SciSat / ACE-FTS (Table 15)
- UARS / HALOE (Table 16)
- ERBS / SAGE-2 (Table 17)
- TIMED / SABER (Table 18)
- Aura /MLS (Table 19)
- Suomi NPP/OMPS-LP (Table 20)

Table 11. Envisat/GOMOS L-2 data required as input to the generation of C3S ozone profiles.

Originating system	GOMOS was on-board the ESA satellite ENVISAT from March 2002 until May 2012. The GOMOS Level 2 data product product (ALGOM2s v 1.0) is generated from the Level 1B product by FMI in the framework of the ESA ALGOM project.
Data class	Earth Observation Data

Sensor type and key technical characteristics	GOMOS (Global Ozone Monitoring by Occultation of Stars) is a medium resolution spectrometer covering the wavelength range from 250 nm to 950 nm. It measures attenuation of stellar light in occultation geometry. Although GOMOS measures during day and night, only dark-limb occultations are used in this project. Ozone profiles are retrieved from UV-Visible atmospheric transmission spectra. Ozone data adequate for atmospheric studies are obtained in the 15–100 km range. The vertical resolution of the retrieved ozone profiles is 2 km below 30 km, 3 km above 40 km, with a linear growth from 2 km to 3 km in the altitude range 30-40 km. It does not depend either on stellar properties or occultation geometry.
Data availability & coverage	GOMOS data are available from May 2002 until December 2011. Until early January 2005, the daily number of measurements was about 400. After July 2005, the number of occultations has been reduced down to ~280 daily. Summer poles are not covered (absence of night-time conditions). Data from May-June 2003, January-July 2005 and February-November 2009 are non-available due to the instrument technical anomalies.
Source data product name and reference to product technical specification documents	GOMOS Level 2 data *[RD-4]*. The ozone ALGOM2s dataset algorithm and data description can be found in *(Sofieva et al., 2017a)*. The ALGOM2s retrievals use IPF V6 data in the middle atmosphere.
Data quantity	The user-friendly gridded ozone dataset is 357 Mb .
Data quality and reliability	The assessment of the GOMOS data quality and reliability is performed part of the GOMOS Quality Working Group activities. The validation and intercomparisons of IPF V6 and ALGOM 2S data can be found in *(Kyrölä et al., 2013; Adams et al., 2014; Hubert et al., 2016; Sofieva et al., 2017a)*.
Ordering and delivery mechanism	Available at https://earth.esa.int/web/sppa/activities/instrument-characterization-studies/algom/data-resources. HARMOZ data are available at the Ozone_cci website (http://www.esa-ozone-cci.org/?q=node/161).
Access conditions & pricing	The team has default access to the GOMOS Level 2 data. The GOMOS Level 2 products are free of charge.
Issues	None.

Table 12. Envisat/MIPAS L-2 data required as input to the generation of C3S ozone profiles.

Originating system	The MIPAS Level-1b data serve as input for several level-2 retrieval processors. Within the project, the KIT/IAA algorithm is used after the round robin exercise performed within the O3CCI project Phase I and is used for the ozone limb vertical profile ECV product.
Data class	Earth Observation Data

Sensor type and key technical characteristics	MIPAS is an infrared limb emission sounder on ENVISAT, designed and operated for measurements of constituents between the upper troposphere and the mesosphere. MIPAS has several observation modes: NOM (6-70 km; 500 km along track-sampling), UTLS (6-50km), MA (18-100km), UA (40-170km), and various others. MIPAS is a rear looking instrument with the lines of sight approximately in the orbit plane. In the original measurement mode, which was operational from July 2002 to March 2004, 17 tangent altitudes between 6 and 68 km were measured per limb scan. Spectral resolution: 0.035 cm-1 unapodized. The altitude of the ENVISAT orbit was about 800 km and the ground track speed is about 510 km per 76.5 s which are needed to record one full limb scan. The field of view covers about 3 km in altitude at the tangent point. The horizontal extension of the field of view is about 30 km at the tangent point. Since January 2005, due to a mirror failure, MIPAS was operating on reduced spectral resolution mode (0.0625 cm-1 unapodized).
Data availability & coverage	MIPAS measures day and night on the altitude range from 6 to 70 km (170 km), pole-to-pole, which gives rise to more than 1000 vertical profiles/day. So far the vmr of 30 trace species, as well as temperature and cloud composition are generated. Global coverage is obtained in approximately 3 days. In current project the complete MIPAS Level 2 V7-240 data are available for Aug-2002 – April 2012 with two modes V7H (High Resolution) and V7R (Reduced Resolution)
Source data product name and reference to product technical specification documents	MIPAS level 1b data (ENVISAT-1 Products Specifications, Vol. 12: MIPAS). MIPAS V7RH_O3-40 +V7H_O3-240
Data quantity	2x5 GB for the O3CCI HARMOZ_ALT and HARMOZ_PRS product
Data quality and reliability	No validation for MIPAS V7 IMK/IAA available.
Ordering and delivery mechanism	MIPAS level-2 data are available from the KIT/IMK/IAA. HARMOZ data are available at the Ozone_cci website (http://www.esa-ozone-cci.org/?q=node/161).
Access conditions & pricing	The team has default access to the MIPAS Level 2 O3CCI data. The MIPAS Level 2 products are free of charge.
Issues	None.

The SCIAMACHY level-2 version 2.9 data (current version, see Table 13) is produced by applying the SCIATRAN radiative transfer model and retrieval package to level 1-b data (see Ozone_CCI ATBD *[RD-22]*) to retrieve the ozone limb vertical profile.

Table 13. Envisat/SCIAMACHY L-2 data required as input to the generation of C3S ozone profiles.

Originating system	SCIAMACHY has been operated on-board the ESA satellite Envisat from March 2002 until May 2012 in a sun-synchronous orbit. SCIAMACHY performs observations in 3 different geometries, i.e., limb, nadir and occultation. The SCIAMACHY level-2 data products are generated from level 1-b data (see Ozone_CCI ATBD *[RD-22]*).
Data class	Earth Observation Data

Sensor type and key technical characteristics	The main difference of the current version (V3.5) with respect to V2.9 (O3CCI_ATBD_Phase1), is the use of different spectral windows and a DOAS (Differential Optical Absorption Spectroscopy) type polynomial fitting in the near UV and visible (Huggins and Chappuis ozone bands). The SCIAMACHY IUP limb retrieval algorithm (V3.5) exploits the scattered radiances in the UV and visible ranges separated in several spectral windows to retrieve ozone number density profiles (window A: 264-274.9 nm, window B: 276.5-287 nm, window C: 289-334 nm, window D 325.5 - 331 nm and window E: 495 - 576 nm) substituting the prior retrieval at discrete wavelengths in the UV and the use of the triplet method in the visible. The ozone number density is retrieved in the altitude range from 8 to 65 km at the measurement grid. The random error for V 3.5 is on the order of 3-5%. The vertical resolution of the SCIAMACHY profile is 3.2 km or lower.
Auxiliary data	The temperature and pressure are derived by using the ECMWF operational stratospheric analysis data (ECMWF). The ground albedo distribution is extracted from the albedo data base from *Matthews (1983)*, a Goddard Institute for Space Studies (GISS) dataset. High precision integrated albedo data at 1°x1° resolution are available for different seasons. The aerosol extinction profiles are taken from the ECSTRA (Extinction Coefficient for STRatospheric Aerosol) model which depends on altitude, latitude and wavelength and is used as input in the retrieval (*Fussen & Bingen, 1999*). This data base was derived from SAGE II solar occultation measurements. Covariance matrices, diagonal elements of the a priori covariance matrix, and averaging kernels are available in addition to the limb ozone profiles.
Data quantity	Approximately 200 MB/day. Total volume of level-2 version 2.9 data is about 700 GB. (Ozone profiles: 34 GB, a priori diagonal elements: ~ 10 GB, covariance matrices: 330 GB, averaging kernels: 330 GB).
Data quality and reliability	Intercomparison of SCIAMACHY IUP limb ozone V3.0 with ozone sonde stations has shown improvements with average differences being below 10% from about 15% in V2.9 *(Jia et al. 2015)*.
Ordering and delivery mechanism	SCIAMACHY level-2 data are available from the Institute für Umweltphysik (IUP) University of Bremen. HARMOZ data are available at the Ozone_cci website (http://www.esa-ozone-cci.org/?q=node/161).

Table 14. Odin/OSIRIS L-2 data required as input to the generation of C3S ozone profiles.

Originating system	OSIRIS (Optical Spectrograph and InfraRed Imaging System) is a Canadian device on board the Swedish satellite Odin that was launched in February of 2001.
Data class	Earth Observation Data

Sensor type and key technical characteristics	Odin has a circular, sun-synchronous orbit, inclined 98° from the equator, at an altitude near 600 km, with a 96 minute period so OSIRIS is very near local dusk on the ascending track and near local dawn on the descending track, going through local midnight near the southern pole and local noon near the northern pole. OSIRIS is a limb-viewing device and the Optical Spectrograph (OS) has a field of view that spans approximately 40km horizontally and 1km vertically. It makes repeated measurements approximately every 2km while scanning up and down between tangent altitudes of about 10 km to 100 km. The scan period is around 1.5 minutes which allows nearly 60 scans every orbit. The OS only sees the summer hemisphere illuminated by the sun, except during the equinoxes when the entire orbit is illuminated. The OS measures 280nm to 810nm with a 1353 pixel-wide CCD, with a spectral resolution of approximately 1 nm. Data from the wavelength range of 475 to 535nm is discarded due to contamination from the spectrograph's order sorter. The InfraRed Imager (IRI) consists of three channels that record the limb radiance at 1260, 1270, and 1530 nm. Each consists of an array of 100 photodetectors with a tangent altitude resolution of about 1 km. The IRI simultaneously measures 100 vertical kilometers in tangent altitude.
Data availability and coverage	OSIRIS Level 2 data covers from 80° S to 80° N for all longitudes. Ozone concentrations are retrieved on a 1km grid from 10.5 km to 59.5 km. The most recent version of OSIRIS Level 2 data product is available from 2002 to 2010. From 2002-2007 Odin's time was shared with other instruments, so OSIRIS was operational for only half time. From 2008-present the other instruments were decommissioned and OSIRIS became operation full time.
Source data product name and reference to product technical specification documents	OSIRIS Level 2 Ozone, documents not available.
Data quantity	The OSIRIS Level 2 data (including aerosol) is currently 5.05 Gb.
Data quality and reliability	Retrieved scans have flags indicating if they are affected by cloud cover, by radiation hits on the instrument detector, or if scans underwent some otherwise unstable retrieval.
Ordering and delivery mechanism	Requests for Odin/OSIRIS data access must go through the ESA data user online registration. HARMOZ data are available at the Ozone_cci website (http://www.esa-ozone-cci.org/?q=node/161).
Access conditions and pricing	Access is free of charge.

The Sub-Millimetre Radiometer (SMR) onboard the Odin satellite, launched in February 2001, makes time-shared limb measurements of strato-mesospheric ozone using several independent bands within the 486-581GHz frequency range. Odin is on a sun-synchronous orbit at about 600km altitude with ~6am/6pm equator crossing time. Measurements of thermal emission lines are performed during day and night and global coverage is achieved during one observation day based on about 15 orbits per day and 45-65 vertical scans between nominally 8 and 70km or 110km per orbit (depending on observation mode). Vertical profiles of ozone and many other species are retrieved using retrieval algorithms based on the Optimal Estimation Method.

The official operational level-2 ozone data are produced by the Chalmers University of Technology in Göteborg, Sweden. The currently recommended version 2.1 ozone data product is measured in a stratospheric mode band centered at 501.8GHz and can be obtained after registration from http://odin.rss.chalmers.se. Ozone data retrieved from other lines are also available. The 501.8GHz v2.1 level-2 product provides stratospheric ozone data in the ~12-50km range with 2.5-3.5km vertical resolution and single-profile precision of about 20%. The systematic error is estimated to be smaller than 0.75ppmv. The Odin data set is available from November 2001 until present. The stratospheric mode measurements relevant here have been performed on every third day until April 2007 and on every other day since then.

Table 15. SciSat/ACE-FTS L-2 data required as input to the generation of C3S ozone profiles.

Originating system	ACE-FTS is on-board the CSA satellite SCISAT which was launched in August 2003, data is available from Feb. 2004 to present. The ACE-FTS level-2 data products (VMR profiles) are generated from the ACE-FTS level 1-b product (infrared limb spectra) at the University of Waterloo.
Data class	Earth Observation Data
Sensor type and key technical characteristics	The ACE-FTS is a high-resolution (0.02 cm-1) Fourier transform spectrometer measuring from 2.2 to 13 µm (750 – 4400 cm-1). It has a circular field of view and uses 2 photovoltaic detectors (InSb and HgCdTe) with a dichroic element to obtain the same field of view. Operating in solar occultation mode, the ACE-FTS provides detailed profiles of the Earth's atmosphere for more than 30 chemical species. More information is available at: http://www.ace.uwaterloo.ca/
Data availability and coverage	ACE-FTS data are available since Feb. 2004 and is still operational. It provides latitudinal coverage from about 85°N to 85°S with complete coverage every 3 months.
Source data product name and reference to product technical specification documents	Current validated version of processing is v3.5/3.6.
Data quantity	Approximately 1 Gb/year (level 2). Total volume is about 8 Gb.
Data quality and reliability	The ACE-FTS team maintains a list of measurements that have known data quality issues.
Ordering and delivery mechanism	ACE is an ESA third party mission and with data available from: http://earth.esa.int/object/index.cfm?fobjectid=3750 HARMOZ data are available at the Ozone_cci website (http://www.esa-ozone-cci.org/?q=node/161).
Access conditions and pricing	The ACE-FTS level-2 products are free of charge.

Table 16. UARS/HALOE L-2 data required as input to the generation of C3S ozone profiles.

Originating system	Halogen Occultation Experiment (HALOE) operated in 1991-2005 on board the Upper Atmosphere Research Satellite (UARS).
Data class	Earth Observation Data
Sensor type and key technical characteristics	Solar occultation. Level -2 data with VMR on pressure grid.
Data availability and coverage	October 1991 – November 2005.

Source data product name and reference to product technical specification documents	HALOE GATTS V19. **HALOE website**.
Data quantity	Harmonized HALOE data: • V19 • File version HARMOZ_PRS fv0003 • File version HARMOZ_ALT fv0001 • 2x177 monthly files with total of 400 MB • Harmonized at UiB-IUP
Data quality and reliability	No filtering applied. Quality has to be determined. Full citation about two problems in profiles: Link to two problems.
Ordering and delivery mechanism	Original data can be downloaded from HALOE GATTS: Download Link HALOE.
Access conditions and pricing	The UARS HALOE level-2 products are free of charge.

Table 17. ERBS/SAGE-2 L-2 data required as input to the generation of C3S ozone profiles.

Originating system	SAGE II (Stratospheric Aerosol and Gas Experiment II) was launched aboard the Earth Budget Satellite (ERBS) in October 1984. The ozone profiles are retrieved in number density (ND) on a geometrical altitude.
Data class	Earth Observation Data
Sensor type and key technical characteristics	Solar occultation.
Data availability and coverage	October 1984 – August 2005.
Source data product name and reference to product technical specification documents	SAGE II V7 - SAGE website - https://asdc.larc.nasa.gov/project/SAGE%20II
Data quantity	Harmonized SAGE II data: • V7 • File version HARMOZ_PRS fv0006 • File version HARMOZ_ALT fv0006 • 2x248 monthly files with total of 600 MB • Harmonized at UiB-IUP
Data quality and reliability	Ozone values during Pinatubo period should be excluded. Full filtering and screening have been applied as recommended by the data provider. See Section 1.2.7.
Ordering and delivery mechanism	https://asdc.larc.nasa.gov/project/SAGE%20II (click on DATA)
Access conditions and pricing	The ERBS SAGE-2 level-2 products are free of charge.

Table 18. TIMED/SABER L-2 data required as input to the generation of C3S ozone profiles.

Originating system	The Sounding of the Atmosphere using Broadband Emission Radiometry (SABER) instrument is one of four instruments on NASA's TIMED (Thermosphere Ionosphere Mesosphere Energetics Dynamics) satellite. It has been launched in Dec. 2001 and is operating.
Data class	Earth Observation Data
Sensor type and key technical characteristics	Infrared Sounder.
Data availability and coverage	January 2002 – December 2018.
Source data product name and reference to product technical specification documents	SABER V 2.0. Website Documentation.
Data quantity	Harmonized SABER data: • V2.0 Channel 96 • File version HARMOZ_PRS fv0003 • File version HARMOZ_ALT fv0001 • 2x157 monthly files with total of 30 GB • Harmonized at UiB-IUP
Data quality and reliability	5 of the files have corrupt time values.
Ordering and delivery mechanism	Download Page. We used the reduced monthly Temp_O3 data via specified ftp server: Link to reduced data sets.
Access conditions and pricing	The TIMED SABER level-2 products are free of charge.

Table 19. Aura/MLS L-2 data required as input to the generation of C3S ozone profiles.

Originating system	Microwave Limb Sounder (MLS) onboard the Aura satellite and part of the A-Train constellation, was launched in 2004. The ozone values are VMR on pressure grid.
Data class	Earth Observation Data
Sensor type and key technical characteristics	Microwave Limb.
Data availability and coverage	August 2004 – December 2018.
Source data product name and reference to product technical specification documents	Product overview MLS.
Data quantity	• V4.2 • File version HARMOZ_PRS fv0005 • File version HARMOZ_ALT fv0004 • 2x137 monthly files with total of 50 GB • Harmonized at UiB-IUP
Data quality and reliability	The filtering applied in the current version following the recommendation of MLS/Aura team.

Ordering and delivery mechanism	https://mls.jpl.nasa.gov/data/
Access conditions and pricing	The MLS AURA level-2 products are free of charge.

Table 20. SUOMI NPP/OMPS L-2 data required as input to the generation of C3S ozone profiles.

Originating system	OMPS-LP is on-board the NASA satellite SUOMI NPP, launched in 2012 and is operational. The OMPS-LP level-2 data products (ozone number density profiles) are generated at the University of Saskatchewan.
Data class	Earth Observation Data
Sensor type and key technical characteristics	The OMPS Limb Profiler measures limb-scattered sunlight in the wavelength range 270—1000 nm employing a prism spectrometer. OMPS-LP images the atmosphere using three vertical slits, one aligned with the orbital plane and the others separated by 250 km at the tangent point on either side of the orbital track. Imaging allows OMPS-LP to obtain along track and vertical sampling of approximately 125 km and 1 km respectively. More information is available at https://earthdata.nasa.gov/earth-observation-data/near-real-time/download-nrt-data/omps-nrt
Data availability and coverage	OMPS data are available since Feb. 2012 and is still operational. It provides ~1600 profiles per day with global coverage.
Source data product name and reference to product technical specification documents	The current version of processing is USask 2D v1.1.0.
Data quantity	Approximately 1 Gb/year (level 2). Total volume is about 8 Gb.
Data quality and reliability	The harmonized dataset (HARMOZ), which contains only valid data, is provided by the University of Saskatchewan. The data from first months of OMPS operation (Feb and March 2012) have lower coverage and possibly some pointing issues.
Ordering and delivery mechanism	OMPS HARMOZ data are available at the Ozone_cci website (http://www.esa-ozone-cci.org/?q=node/161).
Access conditions and pricing	The OMPS-LP level-2 products are free of charge.

2.2 Ancillary data

2.2.1 Surface albedo

Spectral surface albedo data (Table 21) are required as input for the total column and nadir ozone profile retrieval algorithms. These data sets must be available at the UV wavelengths used for the inversion, and at suitable spatial and temporal resolutions.

Table 21. Surface albedo data required for C3S ozone data processing.

Originating system	TOMS, GOME, OMI sensors.
Data class	Climatological data base.
Sensor type and key technical characteristics	Minimum Lambertian Equivalent Reflectivity (MLER) data bases derived from the TOMS, GOME and OMI sensors are available and suitable for nadir UV ozone retrievals.

Data availability & coverage	MLER climatologies are available from TOMS, GOME and OMI. These data sets are specified as global monthly averaged maps, representative for one yearly cycle (i.e. they are distributed in the form of 12 maps for each wavelength interval).
Source data product name and reference to product technical specification documents	The TOMS, GOME and OMI LER climatologies are documented in the following scientific publications: *Herman and Celarier, 1997; Koelemeijer et al., 2003* and *Kleipool et al., 2008*.
Data quantity	The full data base of GOME LER amounts to approximately 100 MB.
Data quality and reliability	The quality of the TOMS, GOME and OMI LER climatologies is documented in the respective scientific publications (see above).
Ordering and delivery mechanism	LER climatologies from relevant sensors are available from the TEMIS web-site - https://www.temis.nl/surface/albedo/ - and from the OMI web-site - https://disc.gsfc.nasa.gov/datasets/OMLER_003/summary.
Access conditions & pricing	Albedo climatologies from TOMS, GOME and OMI are available free of charge.
Issues	None.

2.2.2 Ozone climatology

Ozone vertical profile climatologies are required as input for the total column retrieval algorithms. These data sets must be global in coverage, classified according to the total column and be representative for the main sources of ozone variability in both the troposphere and the stratosphere.

Within C3S_Ozone we use as baseline the total column-classified ozone profile climatology constructed using MLS and sondes measurements (*Labow et al., 2015*) (Table 22) combined with the tropospheric ozone column climatology built using OMI and MLS observations (*Ziemke et al., 2011*) (

Table 23).

Table 22. Ozone profile climatology *(Labow et al., 2015).*

Originating system	Combination of data from MLS and ozone sondes.
Data class	Climatological data base.
Sensor type and key technical characteristics	The *Labow et al.* climatology was formed by combining data from the Microwave Limb Sounder (MLS) with data from balloon sondes. It consists of average ozone profiles for 30° latitude zones covering altitudes from 0 to 60 km (in Z* pressure altitude coordinates).
Data availability & coverage	The climatology is global in scope and available from the web.
Source data product name and reference to product technical specification documents	The ozone profile climatology is fully described in *Labow et al. (2015)*.
Data quantity	Approximately 200 kB.
Data quality and reliability	See *Labow et al. (2015)*.
Ordering and delivery mechanism	The data base is available from the web, e.g. from the TOMS web site - https://directory.eoportal.org/web/eoportal/satellite-missions/t/toms
Access conditions & pricing	The data base is freely available.
Issues	None.

Table 23. Tropospheric ozone column climatology *(Ziemke et al., 2011).*

Originating system	Combination of data from OMI and MLS observations.
Data class	Climatological data base.
Sensor type and key technical characteristics	The *Ziemke et al.* climatology was formed by combining data from the Ozone Monitoring Instrument and the Microwave Limb Sounder. It consists of monthly mean tropospheric ozone columns provided on a grid with a spatial resolution of 1.25° x 1° (Lon x lat) for all latitudes comprised between -60° and + 60°. Corresponding tropopause altitudes are also provided.
Data availability & coverage	The climatology is available from the web (http://acd-ext.gsfc.nasa.gov/Data_services/cloud_slice/).
Source data product name and reference to product technical specification documents	This tropospheric climatology is fully described in *Ziemke et al. (2011)*.
Data quantity	< 10 Mb.
Data quality and reliability	See *Ziemke et al. (2011)* or http://acd-ext.gsfc.nasa.gov/Data_services/cloud_slice/ .
Ordering and delivery mechanism	The data base is available from the web (http://acd-ext.gsfc.nasa.gov/Data_services/cloud_slice/).
Access conditions & pricing	The data base is freely available.
Issues	None.

2.2.3 Digital Elevation Model (DEM)

A global digital elevation model (DEM) is required as input for the total column and nadir profile retrieval algorithms. Within Ozone_cci we use as baseline GTOPO30 DEM (https://www.usgs.gov/science-explorer-results?es=GTOPO30) with a horizontal grid spacing of 30 arc seconds (approximately 1 kilometre) (Table 24).

Table 24. Digital elevation model (DEM).

Originating system	GTOPO30 was derived from several raster and vector sources of topographic information.
Data class	Elevation data base.
Sensor type and key technical characteristics	GTOPO30, completed in late 1996, was developed over a three year period through a collaborative effort led by staff at the U.S. Geological Survey's Center for Earth Resources Observation and Science.
Data availability & coverage	The DEM data is global in scope and available from the web at https://www.usgs.gov/science-explorer-results?es=GTOPO30
Source data product name and reference to product technical specification documents	The GTOPO30 is fully described in the web link.
Data quantity	Approximately 2 Gb.
Data quality and reliability	See Web link.

Ordering and delivery mechanism	The data base is available from the web.
Access conditions & pricing	The data base is freely available.
Issues	None.

2.2.4 Ozone UV absorption cross-sections

Spectroscopic data bases of absorption cross-sections are required as input for the total column and nadir profile ozone retrieval algorithms. Within C3S_Ozone we use as baseline temperature-dependent ozone absorption cross-sections covering the Hartley-Huggins bands from 270 to 340 nm (Table 25).

Table 25. Ozone UV absorption cross-sections.

Originating system	Laboratory data by *Daumont et al. (1992), Malicet et al. (1995)*, and *Brion et al. (1998)*. Laboratory data by *Gorshelev et al. (2014)* and *Serdyuchenko et al. (2014)*.
Data class	Spectroscopic data base.
Sensor type and key technical characteristics	**BDM data set** Absorption cross-sections are measured in the laboratory using a grating spectrometer and an absorption cell. A capacitive manometer measures the pressure of gaseous mixture in the absorption cell all through the experiment. To allow measurement at low temperatures down to 215 K, a two-stage cryostat is used. For details see *Malicet, Brion and Daumont (1989)* and *Daumont et al. (1992)*. ***Serdyuchenko et al.* data set** These new ozone absorption cross-section measurements are performed in the solar spectral region using a combination of Fourier transform and echelle spectrometers. The cross-sections cover the spectral range 213–1100nm at a spectral resolution of 0.02– 0.06nm in the UV–visible and 0.12–0.24nm in the IR at eleven temperatures from 193 to 293K in steps of 10 K. The absolute accuracy is better than three percent for most parts of the spectral region and wavelength calibration accuracy is better than 0.005 nm. For details see *Gorshelev et al. (2014)* and *Serdyuchenko et al. (2014)*.
Data availability & coverage	The data are available from the authors and from public data bases.
Source data product name and reference to product technical specification documents	Laboratory data by *Daumont et al. (1992), Malicet et al. (1995)*, and *Brion et al. (1998)*. Laboratory data by *Gorshelev et al. (2014)* and *Serdyuchenko et al. (2014)* .
Data quantity	BDM: Approximately 10 MB. *Serdyuchenko et al.*: Approximately 36 MB.
Data quality and reliability	See author's references, *Orphal (2003)* and the ESA *Ozone cross-sections review study by J. Orphal*.
Ordering and delivery mechanism	The data base is available from the web.
Access conditions & pricing	The data base is freely available.

Issues	The *Brion, Daumont and Malicet* (BDM) ozone absorption cross-section data set has been recommended for use in remote-sensing applications, notably as part of the activities of the ACSO IGACO-O3 committee (see http://igaco-o3.fmi.fi/ACSO/index.html). However the recent availability of the high quality data set of *Serdychenko et al. (2014)* which covers an extended range of temperatures has motivated new investigations. In comparison to past historical references such as *Bass and Paur (1985)*, these data sets are characterised by (1) improved wavelength registration, (2) more accurate characterization of the temperature dependence of the cross-section, (3) high spectral resolution, and (4) high signal to noise ratio. Although the current baseline for CCI total ozone and ozone profile retrievals in the Hartley and Huggins bands is BDM, the eventual possibility of switching to the new *Serdyuchenko et al.* data set will be investigated.

2.2.5 ECMWF meteorological data

ECMWF meteorological data (Table 26) are needed for the retrieval of ozone data products and for assimilation tools that will be used as one of the approaches to data merging.

Table 26. ECMWF meteorological data.

Originating system	ECMWF (European Center for Middle-range Weather Forecasts) is providing forecasts, up to 10 days ahead, of meteorological parameters to the European Meteorological institutes. Re-analysis of these parameters are also available.
Data class	Meteorological parameters (e.g. temperature, humidity, wind fields, surface pressure, etc.).
Sensor type and key technical characteristics	The ECMWF general circulation model, T1279L91, consists of a dynamical component, a physical component and a coupled ocean wave component. The model formulation can be summarised by six basic physical equations, the way the numerical computations are carried out and the resolution in time and space.
Data availability & coverage	The global data is operationally delivered on a 12 hour basis and can be downloaded by the meteorological institutes via dedicated internet-access.
Source data product name and reference to product technical specification documents	A full set of parameters is available to ECMWF Member States through the operational dissemination system: https://www.ecmwf.int/en/forecasts/datasets As a matter of fact, more parameters are produced and disseminated, than are archived. They are available in Gaussian regular and reduced grid, regular and rotated lat-lon grid forms. Upper air parameters (except humidity) are also available in spectral form.
Data quantity	Approximately 1 Gb per day. Total amount of data at ECMWF is 150 TB.
Data quality and reliability	See web link: http://www.ecmwf.int

Ordering and delivery mechanism	Data is accessible for meteorological institutes of the Member States.
Access conditions & pricing	The data base is only freely available for meteorological institutes of the Member States.
Issues	/

The current status of the usage of ECMWF data sets for generating of the ozone ECV products is summarized in Table 27. As can be seen, most retrieval algorithms make use of meteorological input data, either as a-priori information (when e.g. temperature is retrieved as part of the state vector) or to constrain model parameters used in the inversion process. In addition ECMWF data are also used at KNMI for the assimilation of total ozone columns.

Table 27. Source of meteorological data sets (pressure/temperature) used for generating the C3S_Ozone data products.

Source of PT data / Product	retrieved	climatology	ECMWF data: Operational	ECMWF data: ERA40	ECMWF data: ERA-Interim
Total ozone	X [1]	X			
Nadir ozone profile					X
SCIAMACHY limb ozone profile			X		X [2]
MIPAS ozone profile	X		X [3]		
GOMOS ozone profile			X		
Assimilated ozone products					X

2.2.6 Atmospheric state input to FORLI RTM

2.2.6.1 L1C radiances

FORLI-O_3 v20151001 uses the Level1C radiances disseminated by EumetCast. A subset of the spectral range, covering 1025–1075 cm^{-1}, is used for the O_3 retrieval.

[1] The total ozone algorithm retrieves an effective ozone-weighted mean temperature. A priori T° profiles are taken from the TOMS v8 climatology.

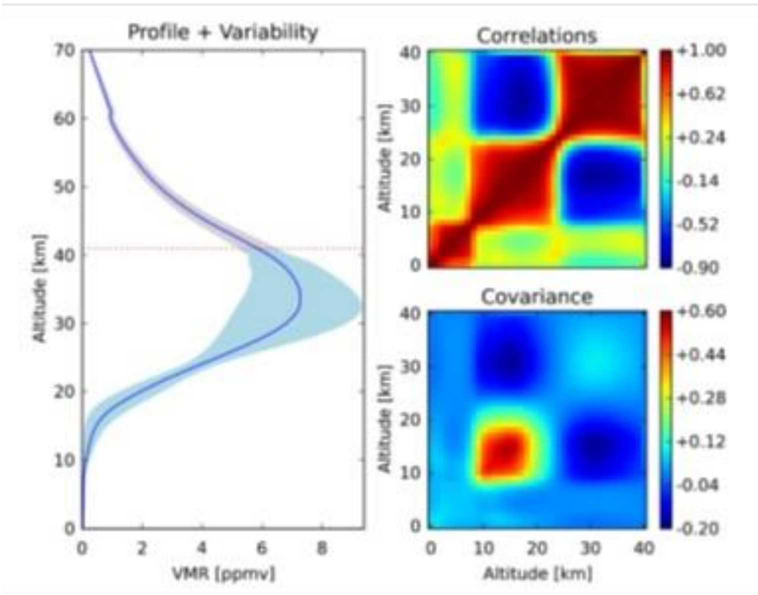
[2] Some of the reprocessed level-2 and level-3 data used ERA-Interim, however there is a limitation in the range of altitude covered by ERA-Interim which prevents its use on a systematic basis.

[3] ECMWF data are used as a-priori in the inversion process.

2.2.6.2 Ozone climatology

The *a priori* profile $\boldsymbol{x_a}$ covariance matrix $\boldsymbol{S_a}$ are constructed from the McPeters/Labow/Logan climatology of ozone profiles (*McPeters, Labow and Logan, 2007*), which combines long term satellite limb measurements (from the Stratospheric Aerosol and Gas Experiment II and the Microwave Limb Sounder) and measurements from ozone sondes. The *a priori* profile $\boldsymbol{x_a}$ is the mean of the ensemble. Figure 1 illustrates this *a priori* information: the *a priori* profile $\boldsymbol{x_a}$ has values slowly increasing from around 25 ppbv at the surface to 100 ppbv at 10km, reaching a maximum of 7.3 ppmv in the middle stratosphere. The variability (taken hereafter as the square root of the variance, i.e. of the diagonal elements of $\boldsymbol{S_a}$) is below 30% in the boundary layer and the free troposphere; it is maximum in the upper troposphere–lower stratosphere, between 10 and 20 km, where it is of the order of 60%. There are significant correlations between the concentrations in the layers 0–10, 10–25 and 25–40 km, but weak correlation between these three (Figure 1).

Figure 1 - Left: $\boldsymbol{x_a}$ (ppmv, blueline) and associated variance (shaded blue) for the FORLI-O3. The dashed red line indicates the top altitude of the last retrieved layer. Right: correlations and $\boldsymbol{S_a}$ variance–covariance matrices in unitless multiplicative factor (from *Hurtmans et al. 2012*).



2.2.6.3 Temperature and humidity profiles

Profiles of temperature and humidity are from the IASI L2 PPF (*August et al., 2012*). The atmospheric temperatures are kept fixed whereas the water profile is used as a priori and further adjusted.

2.2.6.4 Surface temperature

Surface temperatures (land and sea) are from the IASI L2 PPF. Surface temperature is part of the parameters to be retrieved.

2.2.6.5 Cloud fraction

FORLI v20151001 uses the cloud fraction from the IASI L2 PPF. All pixels with a cloud fraction equal to or lower than 13 % are processed.

2.2.6.6 CO_2 profile

A constant vertical profile at 380 ppm is assumed for CO_2.

2.2.6.7 Orography

Orography is from the GTOPO30 global digital elevation model and is integrated in the entire IASI FOV (http://eros.usgs.gov/#/Find_Data/Products_and_Data_Available/gtopo30_info).

2.2.6.8 Emissivity

A wavenumber-dependent surface emissivity above continental surfaces is used while for ocean a single standard emissivity is considered. For continental surfaces it relies on the climatology of *Zhou et al. (2011)*. In cases of missing values in the *Zhou et al.* climatology, the MODIS climatology of *Wan (2008)* is used. It is available on a finer 0.05° x 0.05° grid but is restricted to only 12 channels in the IASI spectral range. In order to deal with this, the spectrally resolved mean emissivity of the Zhou climatology is scaled to match as closely as possible the values in these 12 channels and it is this resulting emissivity that is considered. Finally when there is no correspondence between the IASI FOV and either climatologies, then the mean emissivity of the Zhou climatology is used.

2.2.6.9 Look-up tables

Tabulated absorption cross-sections at various pressures and temperatures are used to speed up the radiative transfer calculation. The spectral range for the LUTs used in v20151001 is 960-1105 cm^{-1} and the spectral oversampling is 100. The absorption cross-sections are computed on a logarithmic grid for pressure from 4.5×10^{-5} to 1 atm with a grid step of 0.2 for the logarithm of pressure, and on a linear grid for temperature (162.8–322.6 K with a grid step of 5K). Relative humidity is also introduced in the LUT, varying linearly between 0 and 100%, by steps of 10%.

2.2.6.10 Spectroscopy

Line integrated absorption cross section, air broadening, self-broadening, line shifting and absorption cross section data are taken from the widely used HITRAN spectroscopic database version 2012 (*Rothman et al., 2013*). Continuum formulations are taken from MT-CKD (*Clough et al., 2005*).

3. Retrieval algorithms and forward models

3.1 Ozone total column retrieval from UV-nadir sensors

Total ozone columns are generally measured from space using earthshine backscattered radiance observations from nadir-viewing instruments. Within C3S, a total ozone climate data record is produced operationally based on the experience built as part of the ESA CCI programme. This data record combines individual regularly extended and updated L2 total ozone data sets from different ESA, ESA Third Party Mission (ESA-TPM) and NOAA/NASA sensors, i.e. GOME/ERS-2, SCIAMACHY/Envisat, GOME-2/Metop, OMI/Aura and OMPS-NM/SNPP. These sensors are described in Sections 1.1.1, 1.1.2, 1.1.3, 1.1.4 and 1.1.5.

3.1.1 Heritage

In the USA, total ozone has been measured since 1978 by NASA and NOAA using a series of TOMS and SBUV instruments *[Bhartia, 2003; Miller et al., 2002]*. In Europe, total ozone measurements from space have been initiated with the GOME instrument, and continued with the successor instruments SCIAMACHY, GOME-2 and OMI. Two different approaches have been used to retrieve total ozone columns from those sensors: DOAS and Direct-fitting.

The DOAS technique for total ozone retrieval was used from the start of the GOME/ERS-2 mission in 1995 (GDP Versions 1-4, see for example *Van Roozendael et al., 2006*), DOAS retrieval is currently implemented in the SCIAMACHY and GOME-2 operational processors, respectively SGP 6.0 *[Lerot et al., 2008]*, GDP 4.7 *[Hao et al., 2014]*. The DOAS technique is fast and provides ozone columns at the 1% level of accuracy in most situations *[Van Roozendael et al., 2006]*.

The Direct-fitting approach provides more accurate total ozone columns, at the cost of slower computational performance. Heritage can be traced back to the analysis of ozone column measurements obtained from the continuous scan Nimbus-7 data *[Joiner and Bhartia, 1997]*. The upgraded GOME operational processor GDP 5 is based on Direct-fitting; the complete 16-year GOME data record has been recently reprocessed *[Van Roozendael et al., 2012]*. The Direct-fitting algorithm GODFIT developed at BIRA-IASB has been further developed as part of the ESA Ozone_CCI activities and has been used to generate L2 total ozone data sets from GOME, SCIAMACHY, GOME-2A/B and OMI with a high level of inter-sensor consistency *[Lerot et al., 2014]*. *Chiou et al. [2014]* have shown that the CCI phase-I GOME, SCIAMACHY and GOME-2 data sets agree at the −0.32 to 0.76% level with the recently published monthly zonal mean total ozone SBUV data. *Koukouli et al. [2015]* have shown that these satellite records agree with ground-based observations at the percent level.

The total ozone production system implemented within C3S inherits directly from the distributed production system developed as part of the CCI programme: individual L2 data sets have been extended and updated at BIRA-IASB using the GODFIT algorithm, and then merged into one single L3 record using the merging algorithm developed at DLR *[Coldewey-Egbers et al., 2015]*.

3.1.2 Level 1 to Level 2

Within C3S, the baseline algorithm for L2 total ozone retrieval from backscatter UV sensors is an updated version of the GOME-type direct-fitting (GODFIT) algorithm jointly developed at BIRA-IASB, DLR-IMF and RT-Solutions for implementation in version 5 of the GOME Data Processor (GDP) operational system. In contrast to previous versions of the GDP which were based on the DOAS method, GODFIT uses a least-squares fitting inverse algorithm including direct multi-spectral radiative transfer simulation of earthshine radiances and Jacobians with respect to total ozone, albedo closure and other ancillary fitting parameters. The basis of the algorithm has been described in detail in the GDP5 Algorithm Theoretical Basis Document *(Spurr et al. 2011)*. More details about description below can also be found in *(Lerot et al. 2014)*, *(Van Roozendael, et al. 2012)* and in the Ozone_cci ATBD *[RD-22]*. This section presents the general features of the algorithm.

3.1.2.1 Overview

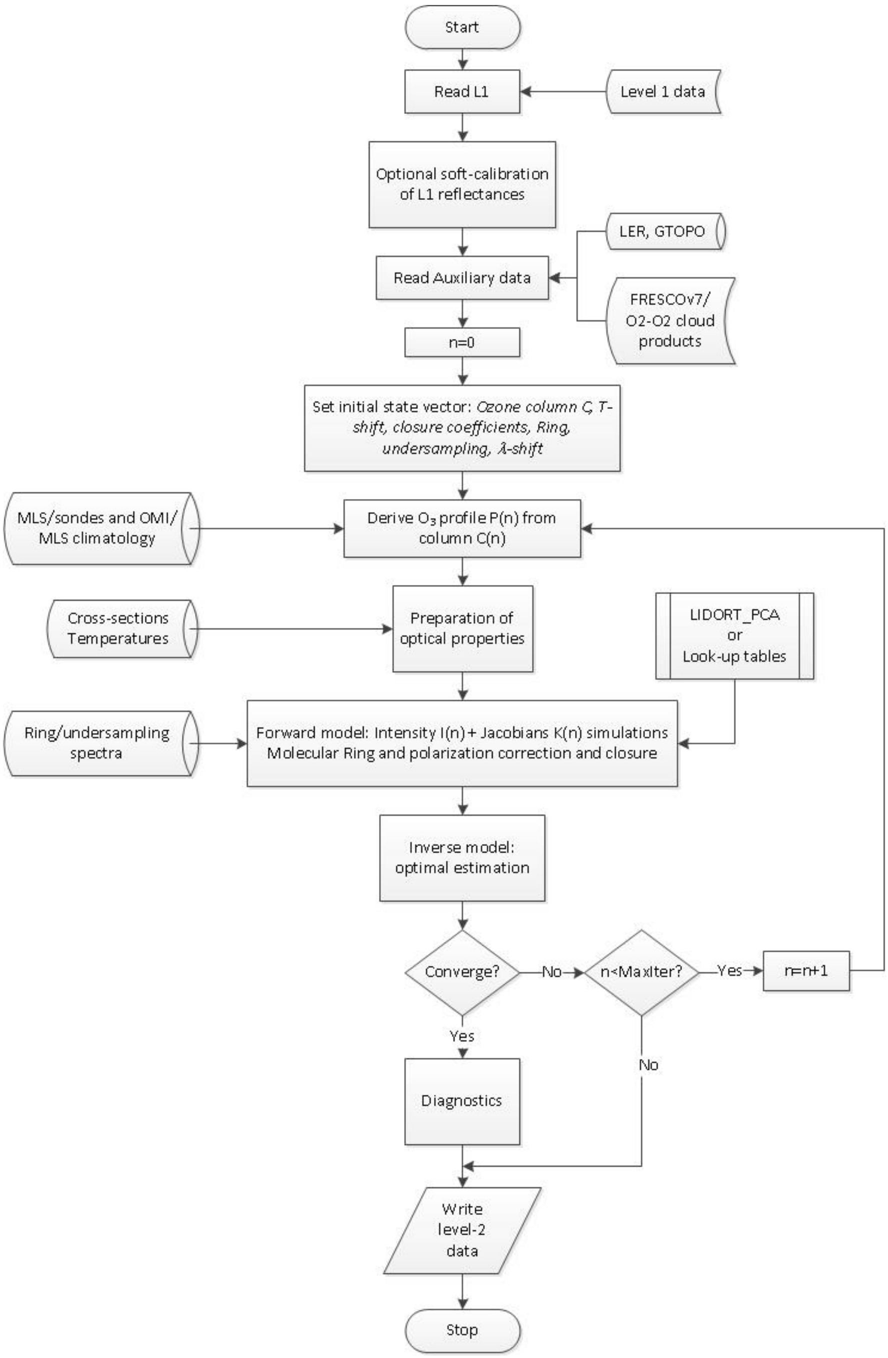
The direct fitting algorithm employs a classical inverse method of iterative least squares minimization which is based on a linearized forward model, that is, a multiple-scatter radiative transfer (RT) simulation of earthshine radiances and associated weighting functions (Jacobians) with respect to state vector elements. The latter are the total ozone column and several ancillary parameters including albedo closure coefficients, a temperature shift, amplitudes for Ring and undersampling corrections, and a wavelength registration shift. On-the-fly RT calculations are done using the LIDORT discrete ordinate model *(Spurr, 2008)*. The performance of the radiative transfer computations has been significantly enhanced with the development of a new scheme based on the application of Principal Components Analysis (PCA) to the optical property data sets *(Spurr et al. 2013)*. Alternatively, the simulated radiances and Jacobians can be extracted from pre-computed tables in order to further accelerate the retrievals. This facilitates greatly the treatment of large amount of data provided by sensors with a very high spatial resolution such as OMI aboard the AURA platform and the future Sentinel-4 and -5(p) instruments.

One specificity of the C3S total ozone L2 processing is that it includes a soft-calibration procedure of the L1 reflectances for some of the sensors considered for the production of the climate L3 merged total ozone data record (see Section 3.1.2.9). This allows to further enhance the inter-sensor consistency between the individual level-2 data sets by empirically correcting for some remaining discrepancies caused by limitations in the calibration and/or instrumental degradation.

Before processing the individual satellite pixels, a recalibration of the L1 irradiance wavelength grid is carried out for each satellite orbit data to have the required very high accuracy for the alignment between the earthshine and reference irradiance spectra on one hand and the cross-sections on the other. This recalibration consists in aligning the solar Fraunhofer lines in the L1 sun spectrum to the position provided by a reference solar atlas *(Chance and Kurucz, 2010)* degraded to the resolution of the instrument. During this procedure, the instrumental slit function can also be characterized in a dynamic way by convolving the reference solar atlas with a predetermined line shape of which key parameters (e.g. the Full Width at Mid-Height) are adjusted simultaneously to the wavelength grid shift parameters. The various cross sections are then convolved dynamically using the slit function fitted during the wavelength calibration. This capability may be particularly useful if the real slit function turns out to differ significantly from the key data slit function or if the instrumental degradation leads to some slit function change over time. Once this is done, total ozone can be inverted for each measured radiance.

The flowchart in Figure 2 gives an overview of the inversion procedure. It is straightforward, with one major decision point. Following the initial reading of satellite radiance and irradiance data (possibly soft-calibrated), and the input of auxiliary data (topography fields, optional temperature profiles, fractional cloud cover and cloud-top-height), the iteration counter is set (n=0), and an initial guess is made for the state vector (total ozone amount, temperature shift, closure coefficients, etc.). A unique ozone profile *P(n)* is then constructed from the total column estimate *C(n)*, using a 1-1 column-profile map based on column-classified ozone profile climatology. For this, we use the climatological database recently released by *Labow et al. (2015)* and constructed using MLS and sondes observations, combined with the tropospheric climatology based on OMI and MLS measurements published by *Ziemke et al. (2011)*. Next, pressure, temperature and height profiles are constructed; this is where the current value of the temperature shift *S(n)* is applied.

Figure 2 - Flow Diagram of the GOME-type direct fitting retrieval algorithm (GODFIT).



The algorithm then enters the forward model step, in which optical properties are created and the LIDORT model called to deliver top-of-atmosphere (TOA) radiances *I(n)*, and the associated ozone column, albedo, T-shift and other weighting functions *K(n)* at each iteration step *n*. These simulated quantities are then corrected for the molecular Ring effect. Next, the inversion module yields a new guess for the ozone column and ancillary state vector parameters. The iteration stops when suitable convergence criteria have been satisfied, or when the maximum number of iterations has been reached (in which case, there is no established convergence and final product). The ozone total column and other parameter errors are computed directly from the inverse variance-covariance matrix.

When the simulated spectra are extracted from a lookup table (LUT) instead of being computed online, the inversion procedure is further simplified. The optical properties do not have to be computed and the calls to the RT model LIDORT are replaced by interpolation procedures through the LUT using directly the state vector variables as input in addition to the geolocation parameters. The radiance LUT was computed using the same forward model as the online scheme in order to have full consistency between the two approaches (see below).

Table 28 lists static and dynamic auxiliary data needed by the retrieval algorithm GODFIT to generate the total ozone ECV. More details are given in Section 2.2 for each of those input data sets.

Table 28. List of auxiliary input needs for generating the total ozone product.

Parameter	Physical unit	Source	Comments
High-resolution solar spectrum	[mol s−1 m−2 nm−1]	*Chance and Kurucz [2010]*	Static
Absorption O_3 cross sections at various temperatures	[cm^2molec.$^{-1}$]	*Serdyuchenko et al., [2014]*	Static
Ring cross-sections	---	Generated internally	Static
Surface Albedo	---	OMI-based monthly LER database *(Kleipool et al. [2008])*	Static Values at 335 nm are used
Surface height	m	GTOPO30 [https://lta.cr.usgs.gov/GTOPO30]	Static Degraded at instrumental resolution
A-priori O_3 vertical profile shapes	DU	Total O_3-classified climatology *(Labow et al., [2015])* combined with the OMI/MLS tropospheric O_3 climatology *(Ziemke et al., [2011])*	Static
Cloud fraction	---	Cloud product FRESCOv7/O2-02 OMI product or extracted from NASA TO3 OMPS product	Dynamic
Cloud top height/pressure	Pa	Cloud product FRESCOv7/O2-02 OMI product or extracted from NASA TO3 OMPS product	Dynamic
Temperature profiles	°K	ECMWF - ERA Interim	Dynamic Only to compute soft-calibration factors.

3.1.2.2 Forward model

Simulation of earthshine radiances and retrieval-parameter Jacobians is done using the multi-layer multiple scattering radiative transfer code LIDORT *(Spurr, 2008)*. LIDORT generates analytic Jacobians for atmospheric and/or surface properties (a.o. Jacobians for total ozone, surface albedo and temperature shift). LIDORT solves the radiative transfer equation in each layer using the discrete-ordinate method *(Stamnes, et al. 1988)*; boundary conditions (surface reflectance, level continuity, direct incoming sunlight at top-of-atmosphere) are applied to generate the whole-atmosphere field at discrete ordinates; source function integration is then used to generate solutions at any desired viewing geometry and output level. The entire discrete ordinate RT solution is analytically differentiable with respect to any atmospheric and/or surface parameter used to construct optical properties *(Spurr, 2002)*, and this allows weighting functions to be determined accurately with very little additional numerical computation.

In addition to the usual pseudo-spherical (P-S) approximation (solar beam attenuation treated for a curved atmosphere) LIDORT also has an outgoing sphericity correction, in which both solar and viewing angles are allowed to vary along the line-of-sight (LOS) path treated for a spherical-shell atmosphere. This approach gives sufficient accuracy[4] for off-nadir viewing geometries (maximum 60°) encountered with polar orbiting sun-synchronous sensors.

A new accelerated-performance scheme for the radiative transfer computation has been implemented within GODFIT. This scheme is based on the application of Principal Component Analysis (PCA) to optical property data sets used for RT simulation – most of the variance in the mean-removed optical data is contained in the first and most important empirical orthogonal functions (EOFs). Thus, full multiple-scattering (MS) computations with LIDORT are done only for the mean profile and the first few EOF optical profiles. These LIDORT MS results are then compared with MS radiances from a 2-stream (2S) RT code *(Spurr and Natraj, 2011)*, and a second-order central difference scheme based on these LIDORT/2S difference and on the data Principal Components is then used to provide correction factors to the MS field at every wavelength. Thus it is only necessary to compute the MS radiances at every wavelength using the much faster 2S code.

LIDORT is a scalar code and therefore polarization is neglected in the RT modeling. Ideally, a vector code such as VLIDORT should be used in the forward model. However, to minimize the computational burden, polarization correction factors are applied to simulated scalar radiances. These factors are extracted from a lookup table of VLIDORT-LIDORT intensity relative differences. This LUT provides correction factors classified according to ranges of the solar zenith, viewing zenith, and relative azimuth angles (from 20 to 85 degrees, 0 to 70 degrees and 0 to 180 degrees respectively), surface altitude (from 0 to 15 km), ground albedo (from 0 to 1) and the total ozone column (from 125 to 575 DU).

3.1.2.3 Atmospheric profiles and the T-shift procedure

In a multilayer atmosphere, the forward model requires the specification of a complete ozone profile. In GODFIT, the ozone profile is parameterized by total column, and latitude. The use of total column as a proxy for the ozone profile was recognized a number of years ago and column-classified ozone profile climatologies were created for the TOMS Version 7 *(Wellemeyer, et al. 1997)*, and Version 8 (V8)

[4] In this context,” accuracy” is the total error of the retrieval.

retrieval algorithms *(Bhartia 2003)*. The same mapping is used for GODFIT with the recent climatology based on MLS and sonde data *(Labow et al., 2015)*. This climatology neglects the seasonal and longitudinal variations of tropospheric ozone. To improve the representativeness of the *a priori* profiles, it is combined with the OMI/MLS tropospheric ozone column climatology *(Ziemke, et al. 2011)*.

Since ozone absorption in the Huggins bands is highly sensitive to temperature, temperature profiles are not only required for hydrostatic balance but also for the determination of ozone cross sections. In GODFIT, a-priori temperature profiles are taken from the monthly zonal temperature climatology supplied with the TOMS Version 8 ozone profiles *(Bhartia 2003)*. In addition, a temperature shift adjustment is being used to improve total ozone accuracy[5] and better reflect the dependence of the ozone absorption signature on temperature at the scale of satellite pixels *(Van Roozendael, et al. 2012)*.

3.1.2.4 Surface and cloud treatment

Lower boundary reflection properties must be specified as an input for the forward model. By default one assumes a Lambertian surface characterized by a total albedo *L*. Most ozone being above the tropopause, clouds can be treated as a first-order correction to the basic ozone retrieval using the independent pixel approximation (IPA). TOA radiance in a partially cloudy scenario is simulated as a linear combination of radiances from clear and fully cloudy scenes, weighted by the effective cloud fractional cover f_c assuming clouds as Lambertian reflecting boundary surfaces. Alternatively, the observed scene can be treated as a single effective surface, located at an altitude resulting from the cloud fraction weighted mean of the ground and cloud altitudes *(Coldewey-Egbers, et al. 2005)*. The effective surface albedo is retrieved simultaneously to the total ozone column using the internal closure mode of GODFIT. We found that this approach minimizes the impact of cloud contamination on the retrieved ozone columns, especially for high clouds and it has been consequently adopted in the current version of the algorithm. By default, cloud optical properties (cloud fraction, cloud top albedo and height) come from the FRESCOv7 algorithm *(Wang et al., 2008)* for GOME, SCIAMACHY and GOME-2 and from the O2-O2 cloud product *(Acarreta et al., 2004)* for OMI or, for OMPS, from the cloud parameters provided in the operational TO3 NASA product *(McPeters et al., 2019)*.

3.1.2.5 Albedo and other forward model closure terms

For internal closure, tropospheric aerosol scattering and absorption and surface reflectivity are brought together in an albedo closure term that is fitted internally, in the sense that coupling between surface and atmosphere is treated properly in a full multiple scattering context. The code thus determines an effective wavelength-dependent albedo in a molecular atmosphere. Assuming that surface albedo *R* is a quadratic or cubic polynomial function, we write:

$$R(\lambda) = \gamma_0 + \sum_{m=1}^{M} \gamma_m (1 - \lambda/\lambda_0)^m \qquad \text{Eq. (1)}$$

We assume first guess values $\gamma_m = 0$ for $m > 0$ and an initial value for γ_0 is taken from a suitable database.

[5] I.e. to diminish the total error of the retrieval.

In order to complete the forward model process, additional effects must be taken into account before simulated intensities can be compared with Level 1b measurements in the inverse model. In particular the Ring effect which shows up as small-amplitude distortions in earthshine and sky spectra due to the effect of inelastic rotational Raman scattering by air molecules *(Grainger and Ring 1962)* must be corrected for. To this aim, we use a revisited semi-empirical formulation including tabulated effective air mass factors and reproducing closely filling-in factors calculated with the LIDORT-RRS radiative transfer code *(Lerot et al., 2014)*.

We then simulate sun-normalized radiances at wavelengths specified by the solar irradiance spectrum supplied with every orbit. There is a wavelength registration mismatch between irradiance and radiance spectra, arising mainly from the solar spectrum Doppler shift; this mismatch varies across an orbit due to changes in the instrument temperature. To correct for this, an earthshine spectrum shift is fitted as part of the retrieval procedure, and this shift value is then an element in the state vector of retrieval parameters. In general, the retrieved spectrum shift value is around 0.008 nm, in line with a Doppler shift. Re-sampling is always done by cubic-spline interpolation.

3.1.2.6 Lookup tables of LIDORT sun-normalized radiances

The goal of the lookup table approach is to replace the online radiative transfer calculation by an interpolation of precalculated radiances. Therefore, we construct a multi-dimensional lookup table of radiances as a function of all varying parameters that enter the LIDORT simulation: the fitted parameters (total ozone column and the ancillary fitting parameters scene albedo and temperature shift), angles describing the observation geometry, surface pressure, as well as latitude, by which we select the appropriate temperature and ozone profile shapes from the TOMSv8 and MLS/sonde climatologies. The tabulated radiances are then calculated for a fixed wavelength grid spanning the 325nm-335nm range at 3 times the instrument sampling rate, using cross sections convolved with the instrument's slit function.

The forward model calculation for a set of parameter values now becomes an interpolation of the radiances at surrounding grid points. For the total ozone column and solar zenith angle, we use quadratic interpolation through 3 surrounding grid points. For the other dimensions of the table, linear interpolation is sufficient. This results in an interpolated radiance as a function of the lookup table's wavelength grid, which is then resampled onto the wavelength grid of the observed spectrum using cubic spline interpolation. The derivative of this interpolation procedure produces the needed Jacobians.

In order to keep the interpolation procedure simple and efficient, the LUT uses a wavelength-independent scene albedo. Within the inversion procedure, only a wavelength-independent albedo is fitted, and the possible wavelength dependence of the spectrally-smooth variation of the measured radiance is taken into account via the fit of a polynomial of which the constant term is neglected.

In order for the lookup table approach to be faster than the online algorithm, frequent hard disk access must be avoided. Because all forward model parameters, except for the time of year, vary rapidly within a single orbit file, this restriction translates into the requirement that the radiances for the full range of those parameters fit in memory. This puts a limit on the density of the table's parameter grid, and some experimentation is necessary to obtain a grid which fits in memory and produces accurate interpolation results over the whole parameter space. To save space, the parameter grid does not include a longitudinal dimension. The precalculated radiances are therefore based solely on the MLS/sonde profile database, which has no longitudinal dependence, and do not take into account the tropospheric climatology OMI/MLS, which would be used in the online approach (section above). After the retrieval, we use the averaging kernels and the difference between the profile used in the lookup table and a more accurate profile which matches the tropospheric column prescribed by the OMI/MLS climatology, to apply a correction to the retrieved total column. Using these techniques, we have managed to construct a lookup table which reproduces the retrieved columns of the online algorithm with an accuracy better than 1%, and a tenfold performance improvement.

3.1.2.7 Inversion scheme

GODFIT is a direct fitting algorithm, using iterative non-linear least squares minimization. In the scientific prototype version mostly used for Ozone_cci work, the optimal estimation inverse method is being used with loose a priori regularization on the state vector elements. The optimal estimation method is well known *(C. D. Rodgers 2000)*; we minimize the quadratic functional cost function:

$$\chi^2 = (y_{meas} - f(x))^T S_y^{-1} (y_{meas} - f(x)) + (x - x_a)^T S_a^{-1} (x - x_a) \qquad \text{Eq. (2)}$$

Here, we have the measurement vector of TOA radiances y_{meas}, the state vector x, the forward model simulations $f(x)$, and the error covariance matrix S_y. x_a is the a priori state vector, with S_a the corresponding covariance matrix. The inversion proceeds iteratively via a series of linearizations about the atmospheric state at each iteration step:

$$x_{i+1} = x_a + D_y[y_{meas} - f(x_i) - K_i(x - x_a)] \qquad \text{Eq. (3)}$$

where:

$$D_y = S_{i+1} K_i^T S_y^{-1} \quad \text{and} \quad S_{i+1} = \left(K_i^T S_y^{-1} K_i + S_a^{-1}\right)^{-1} \qquad \text{Eq. (4)}$$

$K_i = df(x_i)/dx_i$ is the matrix of Jacobians, D_y is the matrix of contribution functions, and S_{i+1} is the solution covariance matrix. The latter is the main diagnostic output. The iteration stops when one or more convergence criteria are met. The computation proceeds efficiently with an SVD (singular value decomposition) on the scaled matrix Jacobians. Since the total ozone inverse problem is not ill-posed, the regularization is only present to ensure numerical stability. The a priori constraints are deliberately made very loose, so that the precision is not compromised in any serious way by a priori smoothing. The a priori vector is taken to be the initial state vector.

3.1.2.8 State vector and inverse model settings

There are typically 7 to 8 elements in the retrieval state vector, listed in Table 29, along with their initial value settings. Aside from total ozone, the algorithm fits the temperature-profile shift parameter, 3 polynomial coefficients for internal albedo closure, 2 amplitudes for the semi-empirical molecular Ring correction and the (optional) undersampling correction and an earthshine spectrum wavelength shift.

Table 29. Summary of fitting parameters for direct fitting total ozone algorithm.

State Vector Element Type	# of parameters	Initial Value
Total ozone (unit: [DU])	1	Previous-pixel
Polynomial Coefficient (Internal Closure)	3	R_{335}, 0.0, 0.0
T-shift (unit: [K])	1	0.0
Ring Fraunhofer	1	1.0
Earthshine Shift (unit: [nm])	1	0.008
Undersampling	1	0.0

The total ozone first guess is taken from the previous pixel value. If this value is not available for some reason, the initial total ozone column is taken from a zonal averaged climatology based on TOMS data *(Stolarski and Frith 2006)*. For closure, the initial value R_{335} is extracted from the surface albedo database at 335 nm as described in Section 2.2.1; other albedo parameters are initialized to zero. Initial values of the under-sampling and T-shift parameters are all zero, while the earthshine shift is initialized to 0.008 corresponding to the average Doppler shift due to the platform speed of around 7000 m/s.

3.1.2.9 Soft-calibration of level-1 reflectances and post-correction of L2 data

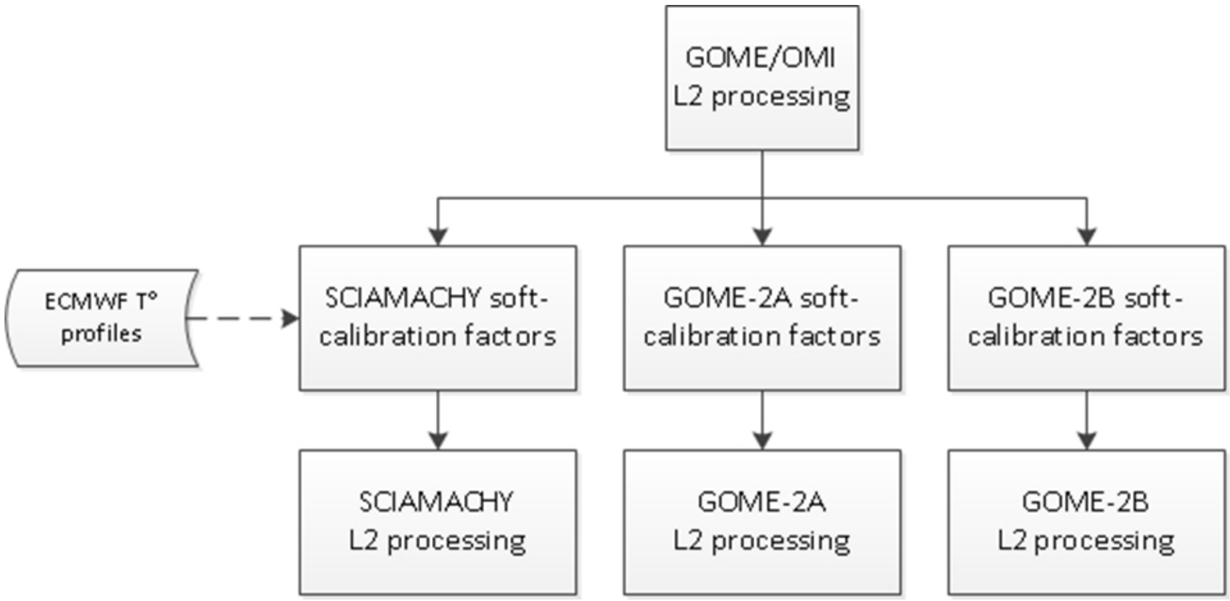
Although a common group of retrieval settings are applied consistently to all level-1 data sets from GOME, SCIAMACHY and GOME-2A/B and OMI, systematic differences between the individual total ozone data sets remain. These originate from systematic radiometric errors and degradation effects affecting the measured level-1 reflectances. To deal with these patterns and enhance the inter-sensor consistency, a soft-calibration scheme has been developed. This procedure relies on comparisons of measured level-1 reflectances to simulated values in the spectral interval 325-335 nm, the simulations being performed with the same forward model as that used for the retrievals.

Experience and validation has shown that level-2 total ozone data sets produced from the GOME and OMI sensors have an excellent temporal stability, are very consistent with each other and also with ground-based instruments without any need for external soft-calibration. Note however that wavelength-independent correction factors need to be applied to the GOME reflectances in the O_3 fitting window if the absolute radiometric calibration is exploited to derive information on the effective reflectivity of the scene. Those corrections factors are derived relatively with respect to measurements carried out at the beginning of the mission over a few reference scenes.

To ensure consistency of the other total O_3 data sets with those two instruments, the GOME and OMI ozone columns in a reference sector in the Pacific Ocean have been used as an external reference to realize the simulations within the soft-calibration scheme. The systematic comparison of the level-1 and simulated reflectances for all satellite observations co-located with the reference O_3 columns allows to identify and characterize possible (broad-band or high-frequency) artefacts in the measured spectra. Based on this analysis, lookup tables (LUTs) of spectral correction factors have been constructed for SCIAMACHY and GOME-2A/B using all computed satellite/simulation reflectance ratios. These LUTs have 3 dimensions: one for the time and two for the viewing and solar zenith angles. Before the total ozone retrieval, the level-1 reflectance is multiplied by the appropriate correction factor spectrum. More details on this soft-calibration scheme are given in *(Lerot et al. 2014)*. In the past, a first version of the initial soft-calibration scheme relied on Brewer measurements. We use now the GOME and OMI data sets as the reference, which allows to restore the independency of the satellite data sets with respect to ground-based observations. The reference needs to be available when reprocessing or updating the L2 data sets requiring a soft-calibration. The production of GOME and OMI total ozone data sets is therefore the first step in the C3S L2 total ozone processing chain as illustrated in Figure 3. Then soft-calibration factors are computed for all other sensors and corresponding L2 data sets are finally produced.

The produced L2 data set from OMPS –NM L1 data shows important “stripes”, i.e. a significant variability of the total ozone column retrieved as a function of the row. Those stripes appear to present a relatively systematic pattern as a function of the row. This is attributed to the coarse spectral resolution of OMPS, leading to an inaccurate spectral wavelength calibration. To circumvent this, a post correction is applied to the retrieved columns by adding systematic offset values, which have been beforehand determined.

Figure 3 - C3S processing chain for generating the L2 total ozone products when soft-calibration of L1 data is required.



3.1.2.10 Averaging kernels

In optimal estimation, the averaging kernel A is defined as the product of the contribution function matrix D_y and the Jacobian matrix K. Generally speaking it is a measure of the departure of the estimator from the truth and the dependence on a priori settings. For the total column retrieval, the problem is well-posed. Accordingly, the averaging kernel matrix reduces to a vector that indicates the sensitivity of the retrieved total column to changes in ozone concentration in different layers. We calculate the averaging kernel as follows. At each wavelength, LIDORT is called to derive the ozone profile layer Jacobians K* using the ozone a priori profile corresponding to the final retrieved total column. The contribution function D_y is obtained making use of the column weighting function K_i calculated as part of the retrieval process. The averaging kernel is then given by $A = D_y K^*$.

When using the LUT approach, calculating the averaging kernels would require that all Jacobians at all wavelengths are stored in a table, too, which would multiply the size of the table, again making it impossible to keep all the required data in memory. Therefore we chose to store precomputed averaging kernels for each grid point, fixing the fitted forward model parameters which are not part of the lookup table grid (closure, Ring amplitude and wavelength shift) at their initial values. We found that this approximation does not have any significant impact.

3.1.2.11 Error budget

Table 30 summarizes our current assessment of the main contributions to the global error budget on total ozone retrieval by direct-fitting. The error budget is given separately in two different regimes, corresponding respectively to low (<80°) and large (>80°) values of the SZA.

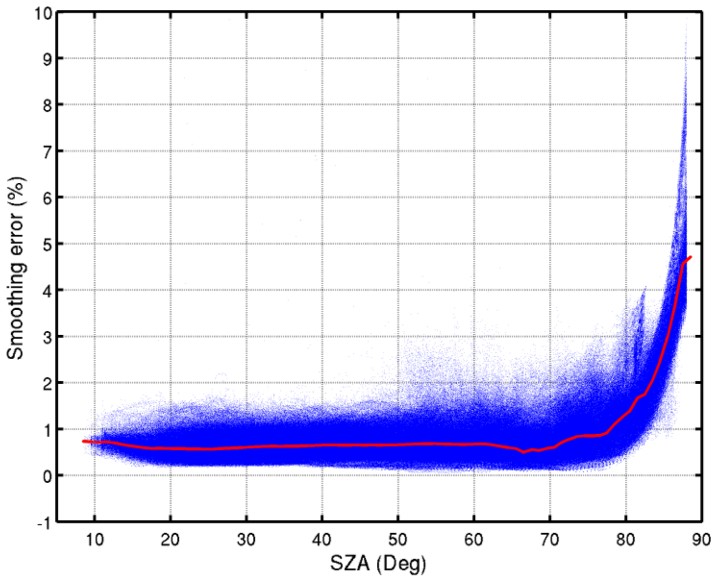
Table 30. Estimation of the error sources of the direct-fitting total ozone retrievals (single pixel retrieval). Pale blue fields indicate random errors, pink fields systematic errors. The errors due to the cloud parameters (orange) are random or systematic depending on the time scale.

Error source	Per cent error	
	SZA < 80°	SZA > 80°
Instrument signal-to-noise	< 0.5	< 2
Soft calibration: Absolute recalibration + structures removal	< 1	< 1.
O_3 absorption cross-sections and its atmospheric temperature	< 2	< 2
Interferences with other species (except in case of volcanic eruption)	< 1.5	< 1
Aerosols (except in case of volcanic eruption)	< 1	< 1.5
O_3 profile shape	< 1	< 5
Cloud fraction	< 0.5	< 0.5
Cloud top height	< 1.5	< 1.5
Total random error (including cloud fields)	**< 1.7**	**< 2.6**
Total systematic error	**< 3.**	**< 5.7**

It includes the random error (or precision) associated with instrument signal-to-noise and which can be derived easily by the propagation of radiance and irradiance statistical errors provided in the level-1 products through the inversion algorithm. It is generally less than 0.5% at moderate SZAs and may reach 2% at SZAs larger than 80°.

The smoothing error associated to the a priori ozone profile shape used in the forward model is assessed using the formalism of Rodgers (*Rodgers, 2000*). Once we have the averaging kernel *A*, the error S_p due to the profile shape may be estimated as $S_p = A^T S_a A$ where S_a is the covariance matrix associated with the *a priori* profile climatology used in the inversion. What is really required here is the covariance associated with the particular retrieved total column for a specific latitude band and season. Covariance matrices associated to the MLS/Sonde climatology have been constructed allowing an estimate of S_p on a pixel-per-pixel basis. As illustrated in Figure 4, the mean total ozone error due to the profile shape is generally less than 1% at low SZAs and is as large as 5% at extreme SZAs.

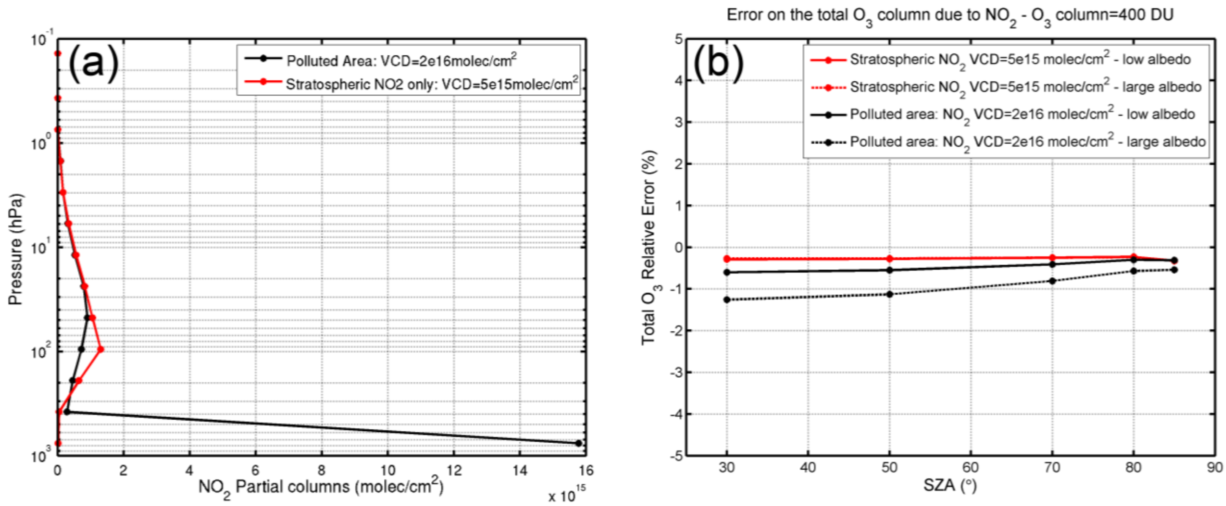
Figure 4 - Mean total ozone error due to a priori O_3 profile shape, as a function of the SZA.



In GODFIT, both absorption by trace gases other than ozone and the impact of aerosols are neglected in the forward model. Here, we estimate the resulting total ozone errors using closed-loop tests. Synthetic radiances are generated using the GODFIT forward model based on optical inputs that include these sources of error (e.g. NO_2 or aerosols). Then, total ozone retrieval is performed using these synthetic spectra and the retrieval settings baseline (i.e. neglecting other trace gases or aerosols in the forward model). The difference with respect to the "true" state gives the error estimate.

To simulate the impact of stratospheric NO_2, a typical stratospheric profile as depicted in Figure 5 has been used to generate synthetic radiances. Total ozone columns retrieved from the resulting synthetic spectra show errors of less than 0.5% for all SZAs and all surface albedos. When considering a profile with a large amount of NO_2 in the lowermost layer (e.g. representative of a heavily polluted scenario), total ozone errors increase slightly but are still less than 0.5% for low surface albedo (0.05). The errors are slightly larger than 1% when the surface albedo is high (0.8), but the likelihood of such a high NO_2 concentration above a bright surface is very small. Similar sensitivity tests have been carried out for BrO and SO_2. The errors due to their neglect are generally negligible, except for a major volcanic eruption scenario with SO_2 column amounts exceeding 50-100 DU. In this case, total ozone errors may reach a few percent.

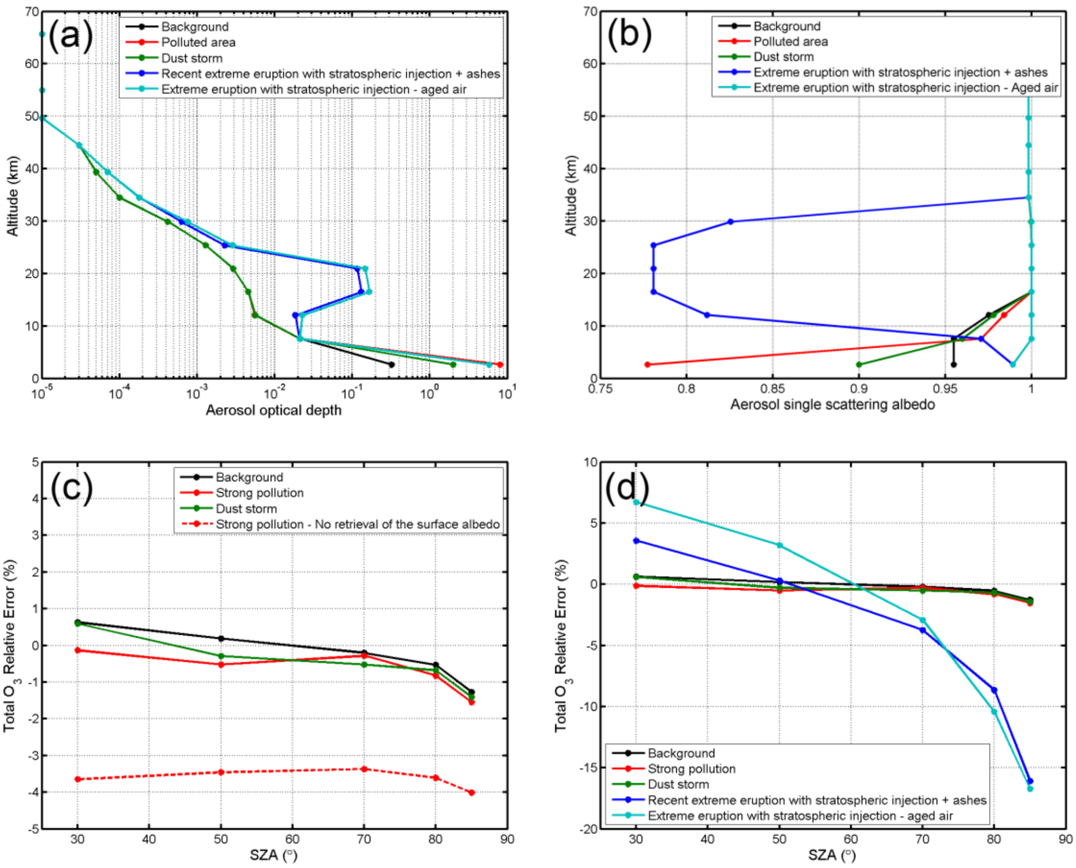
Figure 5 - (a) NO_2 vertical profiles used for generating synthetic radiances. (b) Total ozone error (%) due to neglect of NO_2 in the retrieval scheme, as a function of SZA. For the two profiles shown in (a), ozone errors are plotted for low and high surface albedos (0.05 and 0.8) and for a total ozone column of 400 DU.



The same closed-loop approach has been adopted to estimate the ozone error due to neglect of aerosols in the forward model. A number of scenarios were considered, including a background aerosol case, a heavily polluted scenario with a large amount of absorbing aerosol in the lowermost layer, a dust storm scenario with a large amount of scattering aerosol in the lowermost layer and finally, two scenarios representing major volcanic eruptions with stratospheric injections of absorbing or scattering aerosols. Optical property profiles for these scenarios are plotted in Figure 6 (a-b). The associated total ozone errors, plotted as a function of SZA in Figure 6 (c), are generally within 1%. This small impact is mainly due to the simultaneous fit of the effective surface albedo. As seen in Figure 6 (c) for the pollution scenario, total ozone errors are much larger (up to 4%) if the surface albedo is fixed to a climatological value. This nicely illustrates the added-value of the internal closure mode of GODFIT, which implicitly accounts for tropospheric absorbing and scattering aerosols and avoids relying on the ingestion of highly uncertain external aerosol optical property information. For a scenario with a strong injection of stratospheric aerosols due to a major volcanic eruption such as Pinatubo, the total errors may reach 10% Figure 6 (d).

Other uncertainty estimates have been derived from similar sensitivity tests studies carried out within previous projects (GODFIT A/B, GDP4 and GDP5) or extensively described in *Lerot et al. (2014)*. Total errors are computed assuming all contributions are mutually uncorrelated. The total random errors are estimated to be 1.7 and 2.6 % for the low/moderate and high SZA regimes respectively. The corresponding total systematic errors are less than 3. and 5.7%. Note that this error budget is quite conservative and validation studies show that differences between satellite and ground-based total ozone columns are generally less than 1%.

Figure 6 - (a) Aerosol optical depth and (b) aerosol single scattering profiles used for generating synthetic radiances for a variety of scenarios (see inset and text for more details). (c) Total ozone error (%) due to neglect of aerosols in the retrieval scheme, plotted as a function of SZA for the background, polluted and dust storm scenarios. The red dashed line shows the much larger errors obtained when a fixed (non-fitted) albedo is used. (d) Same as (c) but for strong volcanic eruption scenarios.



3.1.2.12 Output parameters

Level-2 total ozone column data sets derived from the sensors GOME/ERS-2, SCIAMACHY/ENVISAT, GOME-2/Metop-A, GOME-2/Metop-B and OMI/AURA have been processed with the retrieval algorithm GODFIT. The data sets are provided for the complete instrumental time series, under the condition of availability of the input parameters, and are based on the latest level-1 data (see Table 31).

Table 31. Time coverage of the Ozone_cci total ozone level-2 data sets and level-1 versions used in the processing chains.

Platform/Sensor	Time coverage	Level-1 data
ERS-2/GOME	Jul. 1995 – Jun. 2011	ESA L1 v4.00/4.01/4.03
Envisat/SCIAMACHY	Aug. 2002 – Apr. 2012	ESA L1 v8.0x
Metop-A/GOME-2	Jan. 2007 – Nov. 2018	Eumetsat L1 v5.12/6.12
Metop-B/GOME-2	Jan. 2013 – Nov. 2018	Eumetsat L1 v5.12/6.12

Aura/OMI	Oct. 2004 – Jan. 2018	NASA Collection 3
Suomi-NPP/OMPS-NM	Jan 2012 – Jan. 2018	NASA V2.0

There is one ozone column measurement per ground pixel observed by the sensor and the level-2 data sets are distributed via Net-CDF files (one file per orbit). For each measurement, geolocation information, auxiliary and additional fitted parameters, quality indicators, a-priori O_3 profile shape and averaging kernels are also provided in the output files. Table 32 describes the main output variables generated by the level-2 processor.

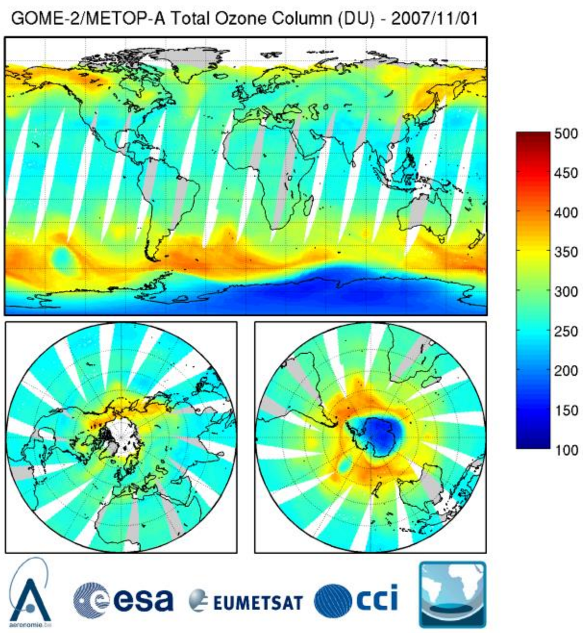
Table 32. Dimension and description of all variables contained in the UV nadir L2 total ozone NetCDF files. N_p represents the total number of measurements for scanning instruments (GOME, SCIAMACHY, GOME-2) and the number of viewing lines for imager instruments (OMI). N_r is the number of rows for imager instruments (60 for OMI; 36 for OMPS), and is 1 for scanner instruments.

Variable Name	Unit	Dimension	Description
total_ozone_column	mol.m-2	N_p x N_r	Retrieved total ozone column
Total_ozone_column_ random_error	mol.m-2	N_p x N_r	Random error associated to the retrieved total column
Total_ozone_column_ smoothing_error	mol.m-2	N_p x N_r	Error due to the a priori profile associated to the retrieved total column
ozone_ghost_column	mol.m-2	N_p x N_r	Partial ozone column comprised between the ground and the effective surface
fitted_ring_coefficient	-	N_p x N_r	Retrieved Ring scaling parameter
effective_temperature	°K	N_p x N_r	Retrieved effective temperature
fitted_state_vector	Various	8 x N_p x N_r	Full fitted state vector (Total O3, T°-shift, 4 polynomial coefficients, Ring scale factor, Radiance wavelength shift)
effective_scene_pressure	hPa	N_p x N_r	Pressure at the effective scene used for the retrieval
effective_scene_albedo	-	N_p x N_r	Retrieved effective albedo of the scene
rms	-	N_p x N_r	Root mean square of fit residuals
reduced_chi_squared	-	N_p x N_r	Reduced chi-square of the fit
nb_of_iterations	-	N_p x N_r	Number of iterations before convergence
convergence_flag	-	N_p x N_r	Convergence flag: 0 for failure, 1 for success

Variable Name	Unit	Dimension	Description
processing_flags	-	N_p x N_r	0: Nominal mode; 1: irregular L1 data - No retrieval; 2: Solar zenith angle larger than 89° - No retrieval; 3: No cloud data - No retrieval; 8: Forward model failure - No retrieval; 9: inversion failure - No retrieval; 21: Pixel affected by row anomaly - No retrieval; 22-24: Pixel might be affected by row anomaly - uncertain output
atmosphere_ pressure_grid	hPa	15 x N_p x N_r	Pressure at levels defining the layers used in the forward model
averaging_kernels	-	14 x N_p x N_r	Averaging kernels in the layers of the forward model
apriori_ozone_profile	mol.m-2	14 x N_p x N_r	A-priori partial ozone columns in the layers of the forward model

Figure 7 shows an example of total ozone columns retrieved from one day of GOME-2/Metop-A observations.

Figure 7 - Total ozone columns retrieved from GOME-2/Metop-A observations on 1st November 2007.

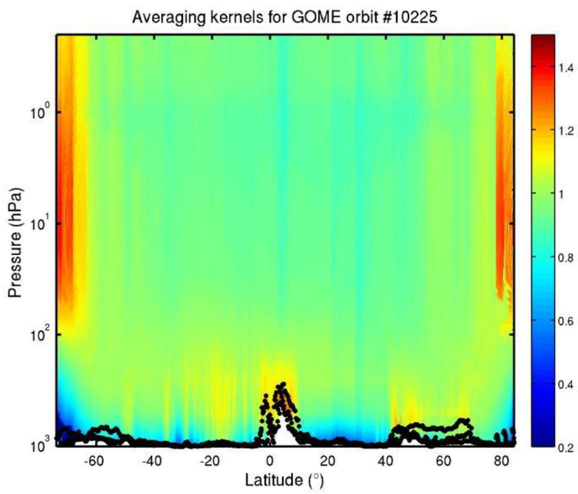


The delivered Net-CDF files contain only measurements for which the convergence has been reached with a number of iterations less than 6 (the typical number of iterations is 3-4). No retrieval is performed for pixels with solar zenith angle larger than 89°. The quality of the total ozone measurements following some specific instrumental operations (e.g. decontamination episodes) may be degraded. These measurements are in general easily detectable and have already been filtered out from the delivered level-2 data sets.

An estimation of the random error is associated to each total ozone column given in the product. This value has been derived via propagation of the level-1 radiance and irradiance statistical errors throughout the inversion algorithm. The reduced chi-squared value is a good indicator of the consistency between the fit residuals and the level-1 errors. Assuming perfectly estimated level-1 errors, the reduced chi-squared will be very close to 1 for a fit without any systematic structures in its residuals. In practice, they are generally ranging between 0.3 and 3. The root mean-squared (RMS) of the fit residuals is another indicator for the fit quality, but does not provide any hint on the nature of the residuals (random or systematic).

As mentioned above, the averaging kernels are also provided for all measurements. They represent the sensitivity of the total column retrieval to a real change in the ozone concentration at a given layer, considering both the observation geometry and the algorithmic features. At low and mid-latitudes, these averaging kernels are generally close to 1 in the stratosphere and upper troposphere and decrease for the lowermost layers, depending on the surface albedo and cloud contamination. At higher solar zenith angles, they change more rapidly with the altitude, making the retrieval quality much more dependent on the a priori profile shape information. Typical averaging kernels are illustrated in Figure 8 for one GOME orbit. The black dots represent the pressure of the effective scene considered for the total ozone retrieval. A smoothing error estimate is also provided in the level-2 files, which represents the impact of the a priori profile shape on the retrieved column. This is computed using both the averaging kernel and the covariance matrices associated to the a priori profile climatology.

Figure 8 - Typical averaging kernels of total ozone retrievals for one GOME orbit. The black dots represent the pressure of the effective scenes considered.



3.1.3 Level 2 to Level 3

3.1.3.1 Total ozone level 3 data from individual sensors

Level 2 ozone column measurements per ground pixel (see Section 3.1.2) serve as input to the level 3 algorithm which is designed to map the level 2 measurements onto a fixed global grid of 1° x 1° in latitude and longitude. This spatial resolution has been selected according to specific requirements of GCOS, IGACO, and WMO for total ozone. Each daily level 3 grid cell contains an average of all level 2 data from the same GMT day that overlap with this cell. Cell values are computed as weighted averages in which the fractional area of overlap of the satellite ground pixel with the given grid cell is used as weight. Level 2 data can be mapped onto more than one grid cell. The daily level 3 gridding algorithm is applied separately to GOME/ERS-2, SCIAMACHY/ENVISAT, GOME-2/Metop-A, GOME-2/Metop-B, OMPS/SNPP and OMI/AURA measurements. The final step is the calculation of monthly means. In order to provide representative values that contain a sufficient number of measurements equally distributed over all days in a month, cut-off values for latitude as a function of month have been defined (see Table 33). In addition to total ozone column information the delivered NetCDF files contain the sample standard deviation, an estimate of the standard error, and the number of measurements used to calculate the monthly mean ozone column. The estimate of the standard error is derived using the standard deviation, the number of measurements, and a multiplicative factor which accounts for the spatial and temporal sampling patterns of the individual sensors. We provide one NetCDF file per month. An overview of the variables (description and dimension) contained in the NetCDF files is given in Table 34 and an overview of the time coverage and update frequency of the individual data sets is presented in Table 35.

Table 33. Cut-off values for latitude as a function of month for the individual and merged UV nadir level 3 monthly mean total ozone products.

Month	Latitudes	Month	Latitudes
January	60.0° N – 90.0° S	July	90.0° N – 57.5° S
February	70.0° N – 90.0° S	August	90.0° N – 62.5° S
March	80.0° N – 80.0° S	September	82.5° N – 72.5° S
April	90.0° N – 65.0° S	October	72.5° N – 85.0° S
May	90.0° N – 60.0° S	November	65.0° N – 90.0° S
June	90.0° N – 57.5° S	December	60.0° N – 90.0° S

Table 34. Dimension and description of the variables contained in the individual and merged UV nadir level 3 total ozone NetCDF files. N_{lat} (=180) is the number of latitudes and N_{lon} (=360) is the number of longitudes.

Variable Name	Unit	Dimension	Description
latitude	degree	N_{lat}	Latitude of grid center
longitude	degree	N_{lon}	Longitude of grid center
total_ozone_column	mol.m-2	N_{lat} x N_{lon}	Monthly mean total ozone column

Variable Name	Unit	Dimension	Description
total_ozone_column_ standard_deviation	mol.m-2	N_{lat} x N_{lon}	Sample standard deviation of mean total ozone column
total_ozone_column_ standard_error	mol.m-2	N_{lat} x N_{lon}	Estimated standard error of mean total ozone column
number_of_measurements	-	N_{lat} x N_{lon}	Number of measurements used to derive the monthly mean total ozone column

Table 35. Time coverage and update frequency of the UV nadir total ozone level 3 data sets.

Sensor/Platform	Time coverage	Update frequency
GOME/ERS-2	Jul. 1995 – Jun. 2011	N/A
SCIAMACHY/ENVISAT	Aug. 2002 – Apr. 2012	N/A
OMI/AURA	Oct. 2004 – now	quarterly
GOME-2/MetOp-A	Jan. 2007 – now	quarterly
OMPS/SNPP	Jan. 2012 – now	quarterly
GOME-2/MetOp-B	Jan. 2013 – now	quarterly
GTO-ECV Merged	Jul. 1995 – now	semi-annually

3.1.3.2 Merged GOME-type total ozone (GTO-ECV)

Within the second phase of ESA's Ozone_cci project an algorithm has been developed by DLR-IMF for the creation of a level 3 monthly mean merged homogeneous total ozone product combining measurements from the five sensors GOME/ERS-2, SCIAMACHY/Envisat, GOME-2/Metop-A, GOME-2/Metop-B, and OMI/Aura. This subsection is dedicated to the illustration of the selected merging approach. A detailed description of the algorithm can also be found in the Ozone_cci ATBD *[RD-22]*, in Coldewey-Egbers et al., 2015, and in Garane et al., 2018. Note that OMPS/SNPP data are not included in GTO-ECV.

Level 3 daily data on a 1°x1° grid from the individual sensors – as described in Section 3.1.3.1 – serve as input to the merging algorithm. In order to minimize the differences between the individual products a so-called inter-satellite calibration approach is applied before assembling the data records. OMI/AURA in combination with GOME/ERS-2 is used as a long-term reference in which GOME has first been adjusted to OMI based on comparisons during the overlap period from 2004 to 2011. Next, SCIAMACHY and both GOME-2 data records are adjusted to this reference. For GOME and SCIAMACHY the correction factors with respect to the reference data set depend on latitude and month of the year, i.e., they are constant for all years. For the GOME-2 sensors an additional time-dependence in the correction factors has been imposed since the differences between GOME-2 and the reference indicate a small drift. For all sensors the calculation of the correction factors with respect to the reference is based on comparing 1° monthly zonal means. These pair-wise monthly zonal means are based on collocated daily 1°x1° data in order to minimize differences due to differences in spatial and temporal sampling. Subsequently the correction factors are applied to daily gridded data in which the correction factors are linearly interpolated in time. Despite of all sensors having different equator crossing times, diurnal changes of ozone are not considered in the calibration approach.

Finally, the five individual data sets are averaged on a daily basis and combined into one single record. The last step is the calculation of monthly means. In order to provide representative values that contain a sufficient number of measurements equally distributed over all days in a month, the same cut-off values for latitude as for the individual level 3 products are used for the merged product (see Table 33). In addition to total ozone column information, the standard deviation, an estimate of the standard error, and the total number of measurements used to derive the monthly mean are provided in the NetCDF files. An overview of the variables (description and dimension) contained in the NetCDF files is given in Table 34. We generate and deliver one NetCDF file per month and the time coverage for the merged product is July 1995 to present. This data product will be updated and extended on a semi-annual basis. Figure 9 shows an example for the merged product (total ozone, standard deviation, and number of available measurements per month) with data from October 2014. Figure 10 shows the total ozone column as a function of latitude and time for the entire period from July 1995 to October 2018.

Figure 9 - GTO-ECV level 3 product for October 2014; left: total ozone column, middle: standard deviation, and right: number of measurements in this month.

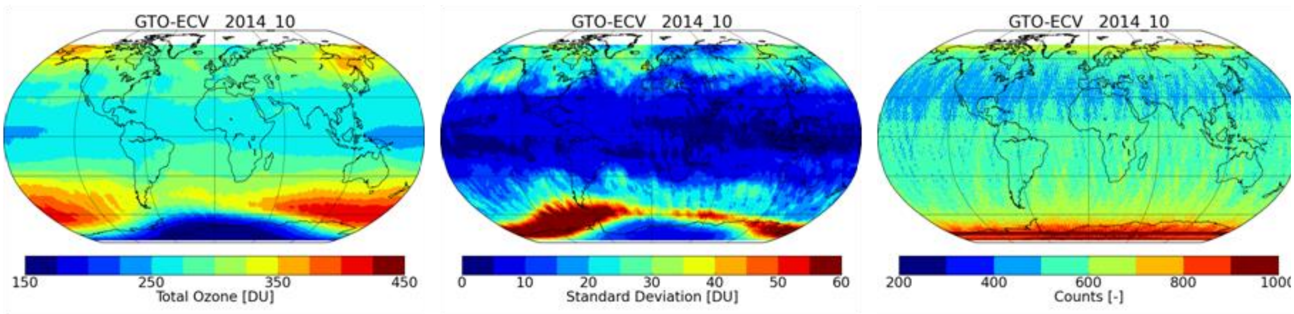
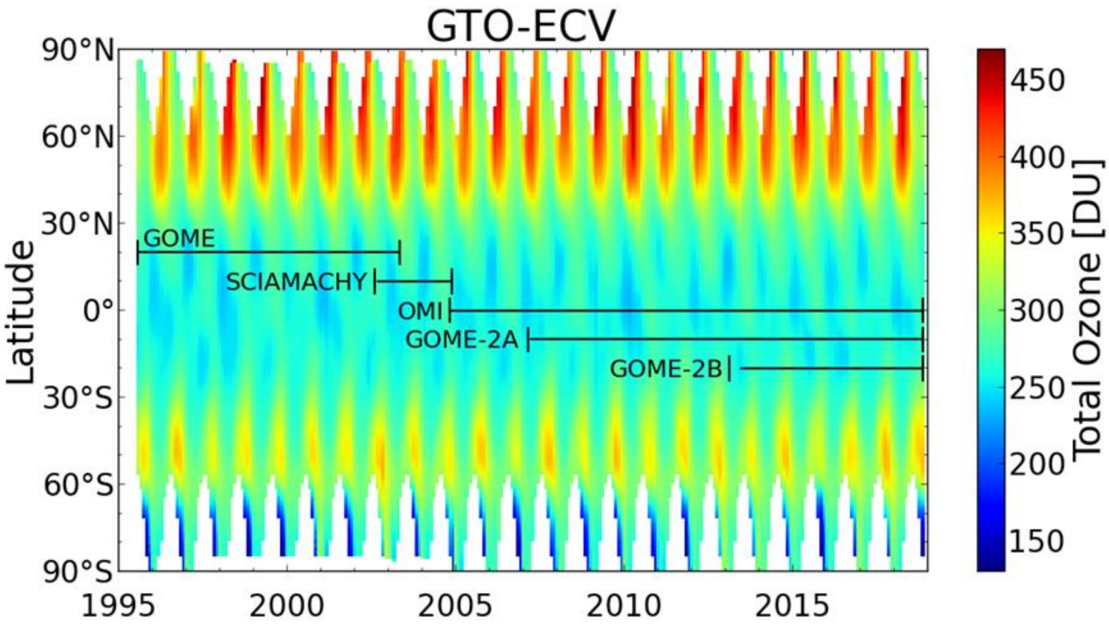


Figure 10 - GTO-ECV level 3 product: total ozone column as a function of latitude and time (07/1995 - 10/2018).



3.1.4 Level 2 to Level 4 – Multi-sensor reanalysis (MSR)

3.1.4.1 Correcting the satellite level 2 dataset

For long-term accuracy and consistency it is crucial to reduce offsets, trends and long-term variations in the satellite data, so that the data can be used as input to the assimilation scheme with minimized biases and with known standard deviations. As in the first version of the ozone multi sensor reanalysis (MSR1), the parameters fitted to correct for the ozone differences (satellite minus ground-based observation) are the Solar Zenith Angle (SZA), the Viewing Zenith Angle (VZA), the effective temperature of stratospheric ozone, time and an offset (with reference year 2000). New compared to the MSR1 correction is the inclusion of a 2nd order SZA correction, since most satellite data sets show a non-linear SZA dependence for low solar elevation angles. A basic assumption is that all corrections are additive to the total ozone amount. By fitting all data together, regional biases that may be caused by offsets of individual ground instruments are avoided. For each satellite product an “overpass” dataset is created for all ground stations and a maximum allowed distance between the centre of the ground pixel and the ground station is defined. This number is typically 50-200 km depending on the ground pixel size. These overpass datasets are fitted to the ground data for the 5 free parameters.

The relevant regression parameters, i.e. those that reduce the RMS (Root Mean Square) between satellite and ground-based observations significantly, are used. The TOMS-EP dataset is corrected for a trend for the last two years only, so this dataset is divided in two. The datasets that show a non-linear dependence on VZA are corrected on a “per pixel” basis. Note that the (S)BUV instruments perform only nadir measurements and the VZA dependence is therefore absent.

Based on the calculated corrections the merged MSR2 level 2 dataset is created. The original satellite datasets were read, filtered for bad data, corrected, and finally merged into a single time ordered dataset. Essential information in the MSR2 level 2 dataset is time, location, satellite id and ozone. In the data assimilation the satellite id is used to assign a corresponding measurement error to this observation. After applying this bias correction procedure, the trend, offset, and seasonal cycle in the satellite observations have been reduced to a negligible level in the MSR2 level 2 data.

3.1.4.2 Ozone model and data assimilation

The chemistry-transport model used is a simplified version of TM5 (*Krol et al., 2005; Huijnen et al., 2010*), which is driven by ECMWF analyses of wind, pressure and temperature fields. The model is using only one tracer for ozone and a parameterization for the chemical modelling. The assimilation approach is an extension of the work described in *Eskes et al., 2005*. As input the assimilation uses ozone column values and estimates of the measurement uncertainty. The ozone model setup and data assimilation scheme in TMDAM have been described in *van der A et al. (2015)*, and we refer to this paper for more details.

3.2 Ozone total and tropospheric column retrieval from IASI

3.2.1 Heritage

The algorithm used for the retrieval of Level-2 ozone data from Level-1 data collected by IASI nadir sensor is described in the Ozone_CCI ATBD *[RD-22]*. In the C3S Ozone project, the Level-2 ozone products serve as input to the generation of Level-3 ozone products (total and tropospheric ozone).

3.2.2 Level 1 to Level 2

The IASI ozone total and tropospheric column products are based on the FORLI (Fast Optimal/Operational Retrieval on Layers for IASI) algorithm v20151001. FORLI is a line-by-line radiative transfer model 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. Validation of IASI total and tropospheric O_3 retrieved from FORLI-O3 v20151001 was carried out by *Boynard et al. (2016, 2018)*. Both papers report a good agreement between total ozone columns retrieved from IASI and UV independent measurements, with IASI slightly higher than UV observations by 1-2 % on average. The comparison with ozone sondes shows that IASI underestimates O_3 by ~10% in the troposphere.

This part describes the methods used for FORLI. Most is extracted from *Hurtmans et al. (2012)*.

3.2.2.1 Basic retrieval equations

For the inversion step, it relies on a scheme based on the widely used Optimal Estimation theory (Rodgers, 2000).

The forward model equation can be written in a general way as

$$y = F(x; b) + \eta \qquad \text{Eq. (5)}$$

where y is the measurement vector containing the measured radiance, x is the state vector containing the molecular concentrations to be retrieved, b represents all the other fixed parameters having an impact on the measurement (temperature, pressure, instrumental parameters...), η is the measurement noise and F is the forward radiative transfer function. The goal of the inverse problem is to find a state vector $\hat{x}$, approximating the true state x, which is most consistent with the measurement and with a certain prior knowledge of the atmospheric state. Specifically, the measured radiances y are combined with an *a priori* state x_a, and both are weighted by covariance matrices representative of their statistical variations, S_η and S_a.

For a linear problem, the retrieved state, solution of the Optimal Estimation, is given by

$$\hat{x} = x_a + \left(K^T S_\eta^{-1} K + S_a^{-1}\right)^{-1} K^T S_\eta^{-1} (y - K x_a) \qquad \text{Eq. (6)}$$

where K is the Jacobian of the forward model F, the rows of which are the derivatives of the spectrum with respect to the retrieved variables.

3.2.2.2 Assumptions, grid and sequence of operations

3.2.2.2.1 Spectral ranges

FORLI-O_3 v20151001 uses the Level 1C radiances disseminated by EumetCast. A subset of the spectral range, covering 1025–1075 cm^{-1}, is used for the O_3 retrieval. The spectral range used in the forward model is 960-1105 cm^{-1} and the spectral oversampling is 100.

3.2.2.2.2 Vertical grid

FORLI-O3 uses a vertical altitude grid in km.

3.2.2.2.3 Ozone state vector

The ozone product from FORLI is a profile retrieved on 40 1km-thick layers between surface and 40 km, with an extra layer from 40 km to TOA.

3.2.2.2.4 Other state vector elements

Besides the ozone profile, surface temperature and the water vapour column are retrieved.

3.2.2.2.5 Measurement covariance matrix

S_η is taken diagonal. The value of the noise is wavenumber dependent in the spectral range used for the retrieval, varying around 2 x 10^{-8} W/(cm^2 cm^{-1} sr).

3.2.2.2.6 Iterations and convergence

We assume a moderately non-linear problem, where Eq. (6) is iteratively repeated using a Gauss-Newton method until convergence is achieved. For iteration j :

$$x_{j+1} = x_a + \left(K_j^T S_\eta^{-1} K_j + S_a^{-1}\right)^{-1} K_j^T S_\eta^{-1}\left[y - F(x_j) + K(x_j - x_a)\right] \qquad \text{Eq. (7)}$$

The gain matrix G is the matrix whose rows are the derivatives of the retrieved state with respect to the spectral points. From Eq. (6), it can be shown that

$$G = \left(K^T S_\eta^{-1} K + S_a^{-1}\right)^{-1} K^T S_\eta^{-1} \qquad \text{Eq. (8)}$$

Convergence is achieved when

$$d_i^2 = [F(x_{i+1}) - F(x_i)]^T S_{\delta\hat{y}}^{-1} [F(x_{i+1}) - F(x_i)] \ll m \qquad \text{Eq. (9)}$$

where $S_{\delta\hat{y}} = S_{\grave{o}}\left(\hat{K} S_a \hat{K}^T + S_{\grave{o}}\right)^{-1} S_{\grave{o}}$ and m is the degree of freedom.

3.2.2.3 Radiative Transfer Model (RTM)

3.2.2.3.1 General formulation

3.2.2.3.1.1 Ray tracing for upward flux

The Ray-tracing defines for off-nadir geometries the path s versus the altitude z. This path depends on the zenith angle of the beam (θ) as seen from the surface, which, under the approximation of a flat atmosphere, is equal to $\sec\theta$. Although the plane-parallel approximation could reasonably be applied for IASI at near-nadir, it is not adapted at larger viewing angles. The spherical shape of the Earth is explicitly accounted for in FORLI by including a local radius of curvature for the Earth $R_\oplus$ and the index of refraction of air. The elementary path is then written as

$$ds = \frac{n(z)(z + R_\oplus)dz}{\sqrt{n^2(z)(z + R_\oplus)^2 - R_\oplus^2 n^2(z_G)\, sin\,\theta}} \qquad \text{Eq. (10)}$$

where $n(z)$ is the index of refraction of air at altitude z. The altitude dependency is expressed through the variation of temperature, pressure and humidity and is modelled using the Birch and Downs formulation (*Birch and Downs, 1994*). The index of refraction is considered constant in the IASI spectral range. In order to calculate the path along the line of sight, Eq. (5) is integrated using a numerical method, as no analytical closed form exists.

3.2.2.3.1.2 Radiative transfer

Local thermodynamic equilibrium is assumed. The monochromatic upwelling radiance at TOA is then calculated as

$$L^\uparrow(\tilde{\nu};\theta,z) = L^\uparrow(\tilde{\nu};\theta,0)\tau(\tilde{\nu};\theta,0,z) + \int_0^z J(\tilde{\nu},\Omega,z')\frac{\partial}{\partial z'}\tau(\tilde{\nu};\theta,z',z)dz' \qquad \text{Eq. (11)}$$

where $L^{\uparrow}(\tilde{v};\theta,0)$ is the radiance at the start of the light path (i.e. that of the emitting surface) at wavenumber $\tilde{v}$ with a ground zenith angle θ, $\tau(\tilde{v};\theta,z',z)$ is the transmittance from altitudes z' to z, and $J(\tilde{v},\Omega,z')$ is the atmospheric source term which depends on both thermal emission and scattering.

For FORLI, only clear or almost-clear scenes (cloud fraction in the field--of--view (FOV) lower than typically 20%; see specific documents for CO, O_3 and HNO_3 for threshold values) are analyzed and the atmosphere is therefore considered as a non-scattering medium. In that case J becomes independent on geometric angle, thus simplifying to the black-body emission function $B(\tilde{v},T)$.

The transmittance $\tau(\tilde{v};\theta,z',z)$ in Eq. (11) is related to the absorption coefficient κ by

$$\tau(\tilde{v};\theta,z',z) = exp\left[-\int_{z'}^{z}\sum_{j}\kappa_j(\tilde{v};z'')\rho_j(z'')\frac{\partial s(\theta,z'')}{\partial z''}dz''\right] \qquad \text{Eq. (12)}$$

where j refers to a given gaseous species, $\rho_j(z'')$ is the molecular density of that species at altitude z'', and $s(\theta,z'')$ is the curvilinear path determined by the ray tracing. The absorption coefficient κ contains absorption features described by single spectral lines; regions affected by absorption of heavier species (where cross-sections would need to be used) are avoided. Also absorption continua are explicitly considered in the calculation of κ.

A precise calculation of the Earth's source function $L^{\uparrow}(\tilde{v};,\theta,0)$ in Eq. (11) has to be achieved to properly model the spectrum recorded at TOA. That term is basically governed by the black-body emission of the ground surface, modified, however, by the emissivity and reflectivity of that surface. Considering a surface of emissivity $\grave{o}(\tilde{v})$:

$$L^{\uparrow}(\tilde{v};\theta,0) = \grave{o}(\tilde{v})B(T_{skin}) + (1-\grave{o}(\tilde{v}))L_0^{\downarrow\dagger}(\tilde{v}) + \alpha(\tilde{v})L_0^{\downarrow\mathring{a}}(\tilde{v}) \qquad \text{Eq. (13)}$$

where $B(T_{skin})$ is the ground black-body Planck function at the ground temperature T_{skin} ;

$$L_0^{\downarrow\dagger}(\tilde{v}) = \frac{1}{\pi}\int_0^{2\pi}d\varphi\int_0^{\pi/2}d\theta L_0^{\downarrow}(\tilde{v};\theta)\sin\theta\cos\theta \qquad \text{Eq. (14)}$$

is the mean radiance associated to the total downward flux reaching the surface, integrated upon all the geometries considering a Lambertian surface; $\alpha(\tilde{v})L_0^{\downarrow\mathring{a}}(\tilde{v})$ is the fraction of sun light that is retro-reflected in the direction of the sounding beam, which depends on the sun azimuthal angle and the surface effective reflectivity $\alpha(\tilde{v})$. In FORLI both contribution from Lambertian and specular reflections are explicitly taken into account, following

$$\alpha(\tilde{v}) = \left((1-\grave{o}(\tilde{v}))\mu_{\delta 0} + \rho\mu_{glint}\right)6.7995\times10^{-5} \qquad \text{Eq. (15)}$$

with

$$\mu_{\delta 0} = \frac{\cos \theta^{å}}{\pi} \qquad \text{Eq. (16)}$$

and

$$\mu_{glint} = \frac{\cos \theta + \cos \theta^{å}}{\sqrt{2[1 + \sin \theta^{å} \sin \theta \cos(\varphi - \varphi^{å}) - \cos \theta \cos \theta^{å}]}} \qquad \text{Eq. (17)}$$

Where θ, $\theta^{å}$, φ and $\varphi^{å}$ are the sun and satellite zenithal and azimuthal angles respectively, and where ρ in Eq. (15) is the effective reflectivity for specular reflection; the last factor on the right hand side of that equation is the sun solid angle. Note that $L_0^{\downarrow å}(\tilde{\nu})$ in Eq. (13) is modeled by a Planck blackbody function at 5700 K, without including spectral lines.

3.2.2.3.2 Numerical approximations

In order to perform the radiative transfer calculation, a discretized layered atmosphere has to be considered. Typically a 1 km-layered atmosphere is assumed. The convention adopted here is to label the levels from 0 to N N for altitudes starting from ground to the TOA, with an atmospheric layer bounded by two levels. The layer index is then ranging from 1 to N. For each layer, average parameters (e.g. $\bar{T}_i$, $\bar{P}_i$, …) are computed.

3.2.2.3.2.1 Ray tracing

Eq. (10) is integrated for each layer using a Gauss-Kronrod quadrature scheme. For each layer, the partial column of each molecule j is also computed using

$$PC_{i,j} = \int_{z_i}^{z_{i+1}} \rho_j(z) \frac{ds(z)}{dz} dz \qquad \text{Eq. (18)}$$

where $\rho_j(z)$ is the molecular density (in molecule/cm^3).

3.2.2.3.2.2 Radiative transfer

Assuming clear sky, Eq. (11) is discretized using a recursive representation evaluated successively for each layer $i = 1, \dots, N$:

$$L_i^{\uparrow} = \bar{B}_i + \left(L_{i-1}^{\uparrow} - \bar{B}_i\right)\tilde{\tau}_i \qquad \text{Eq. (19)}$$

where $\bar{B}_i$ is the average constant Planck function for layer i computed at the average temperature $\bar{T}_i$ of that layer and $\tilde{\tau}_i = \tau(\tilde{\nu}, z_i, z_{i-1})$ is the effective transmittance of that layer. $L_0^{\uparrow}$ is evaluated using successively two recursions similar to Eq. (13), the first being to approximate the downward flux $L_0^{\downarrow\dagger}(\tilde{\nu})$. The evaluation of this equivalent downward flux integral in Eq. (19) is simplified by computing an effective downward radiance with a zenith angle of 53.5°, which approximates the integral within a few percent *(Elsasser, 1942; Turner et al., 2004)*. Accordingly, the computational cost gain is made at a minor error cost in most situations.

Effective transmittances are computed for each layer using a formulation close to the analytical form Eq. (15), but using the average parameters:

$$\tilde{\tau}_i = exp\left[-\sum_j PC_{i,j} \sum_l \kappa_{j,l}(\tilde{\nu}; \bar{T}_i, \bar{P}_i)\right] \quad \text{Eq. (20)}$$

where i refers to the layer; j, to the molecular species; and l, to the spectral line when relevant. For water vapour, the water concentration enters in the line shapes definition, and we should rigorously write $\kappa_{j,l}(\tilde{\nu}; \bar{T}_i, \bar{P}_i, VMR_{j,l})$.

A special feature of FORLI is to work with unitless multiplying factors $M_{i,j}$ instead of the partial columns $PC_{i,j}$ themselves. The multiplying factors are calculated with respect to the *a priori* profiles, except for water vapour for which the level 2 first guess retrieved at EUMETSAT CAF *(August et al., 2012)* is used instead. Therefore Eq. (20) becomes

$$\tilde{\tau}_i = exp\left[-\sum_{j=fitted} M_{i,j} PC_{i,j} \sum_l \kappa_{j,l}(\tilde{\nu}; \bar{T}_i, \bar{P}_i) - \sum_{j=fixed} PC_{i,j} \sum_l \kappa_{j,l}(\tilde{\nu}; \bar{T}_i, \bar{P}_i)\right] \quad \text{Eq. (21)}$$

where the sum runs over the fitted molecules and the j-fixed molecules.

The total state vector ends up to be all the multiplying factors $M_{i,j}$ and all the non-molecular parameters (ground temperature T_{skin}, emissivity or spectral/radiometric calibration parameters) that have to be adjusted. Specifically in FORLI, only $M_{i,j}$ (the trace gas profile and the water vapour column) and T_{skin} are retrieved.

3.2.2.4 Error description

The fitted variance-covariance matrix $\hat{s}$, representing the total statistical error after the retrieval, is written

$$\hat{s} = \left(K^T S_\eta^{-1} K + S_a^{-1}\right)^{-1} \quad \text{Eq. (22)}$$

It includes the contribution from the smoothing error and the measurement error, which can be decomposed according to *Rodgers (2000)*.

Averaging kernels are calculated as

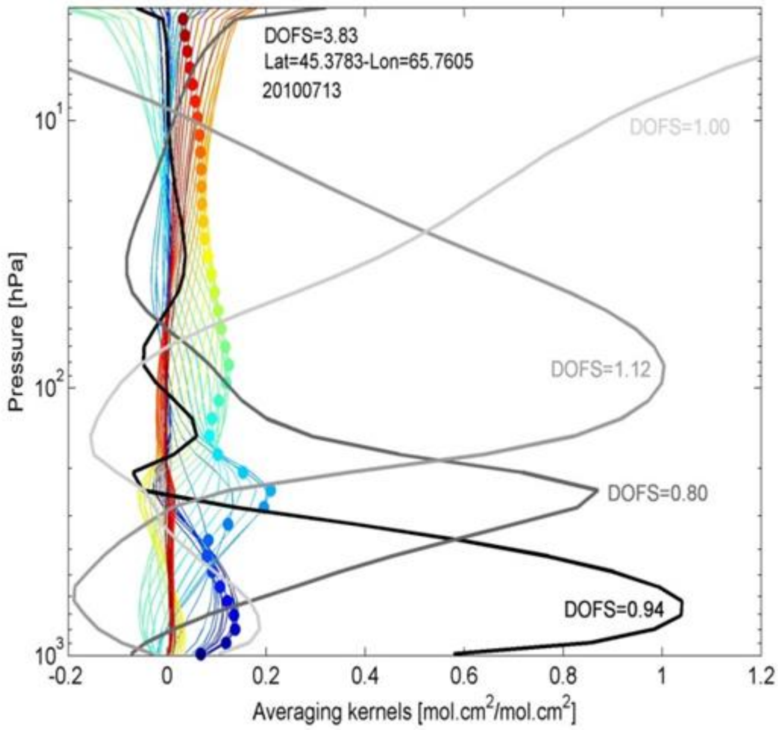
$$A = GK \quad \text{Eq. (23)}$$

where

$$G = \left(K^T S_\eta^{-1} K + S_a^{-1}\right)^{-1} K^T S_\eta^{-1} \quad \text{Eq. (24)}$$

Typical averaging kernels are represented in Figure 11.

Figure 11 - Example of averaging kernels for FORLI-O3 retrievals.



3.2.2.5 Output product description

Level-2 total ozone data sets derived from the sensors IASI/Metop-A and IASI/Metop-B have been processed with the FORLI v20151001 retrieval algorithm. The data sets are provided for the complete instrumental time series, under the condition of availability of the input parameters, and are based on the Level 1C radiances disseminated by EumetCast.

The format of the Level 2 ozone profile product file from the FORLI algorithm is NetCDF. The FORLI algorithm for IASI operates with multiplication factors, with the a priori as reference, and the profile is adjusted in layer partial columns. The original output profile is in partial columns but is provided here in the units needed to follow the general convention. The values in all groups are taken from the level 1 or other input data files, or calculated by the program. Further details on ancillary data, can be found in Section 2.2.6.

There is one ozone profile measurement per ground pixel observed by the sensor and the level-2 data sets are distributed via Net-CDF files (one file per day). For each measurement, geolocation information, auxiliary and additional fitted parameters, quality indicators (to be defined yet), a-priori

O_3 profile shape and averaging kernels are also provided in the output files. Table 36 describes the main output variables generated by the level-2 processor.

Table 36. Dimension and description of all variables contained in the IASI L2 ozone NetCDF files. N_{obs} represents the total number of IASI measurements. N_{layers} is the number of retrieval vertical layers and $N_{pressures}$ is the number of retrieval pressure levels.

Variable Name	Dimension	Unit	Description
latitude	N_{obs}	degree	latitude of the ground pixel center
longitude	N_{obs}	degree	longitude of the ground pixel center
time	N_{obs}	NA	hour in the day as hhmmss
sun_zen_angle	N_{obs}	degrees	solar zenith angle at the Earth's surface for the pixel center
satellite_zen_angle	N_{obs}	degrees	MeOp zenith angle at the Earth's surface for the pixel center
orbit_number	N_{obs}	NA	MetOp orbit number
scanline_number	N_{obs}	NA	scaline number in the MetOp orbit
pixel_number	N_{obs}	NA	pixel number in the current scanline
cloud_cover	N_{obs}	percent	Eumetsat total cloud coverage in the IASI pixel
dofs	N_{obs}	NA	degrees of freedom of the signal in the retrieved ozone partial column profile
retrieval_quality_flag	N_{obs}		retrieval quality flag summarizing processing flags (to be defined and for the moment, 0 for all observations)
surface_altitude	N_{obs}	m	altitude of the surface
tropopause_altitude	N_{obs}	m	altitude of the tropopause
thermal_contrast	N_{obs}	K	thermal contrast
ozone_total_column	N_{obs}	mol m^{-2}	retrieved ozone total column in mole/m2
ozone_partial_column_profile	N_{obs} x N_{layers}	mol m^{-2}	retrieved ozone partial column vertical profile in mole/m2 in the layers defined by the levels given in the variable atmosphere_pressure_grid
ozone_partial_column_error	N_{obs} x N_{layers}	mol m^{-2}	vertical profile of total retrieval error associated to ozone partial column vertical profile in the layers defined by the levels given in the variable atmosphere_pressure_grid
ozone_apriori_partial_column_profile	N_{obs} x N_{layers}	mol m^{-2}	ozone a priori partial column vertical profile in mole/m2 and in the layers defined by the levels given in the variable atmosphere_pressure_grid
air_partial_column_profile	N_{obs} x N_{layers}	mol m^{-2}	air partial column vertical profile in mole/m2 in the layers defined by the levels given in the variable atmosphere_pressure_grid

Variable Name	Dimension	Unit	Description
atmosphere_pressure_grid	N_{obs} x $N_{pressures}$	hPa	pressures in hPa corresponding to levels used to define inversion layers: 40 layers of about 1 km height between Earth's surface and 40 km with an additional layer from 40 km to the top of the atmosphere
averaging_kernels_matrix	N_{obs} x N_{layers} x N_{layers}	DU/DU	ozone partial column averaging kernels matrix (DU/DU) in the layers defined by the levels given in the variable atmosphere_pressure_grid

3.2.2.6 Retrieval and quality flags

The IASI L2 data were filtered out in order to keep only O_3 measurements characterized by a good spectral fit based on quality descriptive and fit flags implemented in FORLI. All data meeting the following quality flags were rejected:

Descriptive flags:

- if there is an error related to the L1C data
- if T, H_2O, cloud L2 data associated to L1C data are missing
- if H_2O L2 profile is incomplete or if the skin pressure is missing
- if a partial O_3 column is negative
- if skin temperature is unrealistic

Fit flags:

- if the spectral fit residual root mean square (RMS) is higher than 3.5×10^{-8} W/(cm^2 sr cm^{-1})
- if the spectral fit residual bias is lower than -0.75×10^{-9} W/(cm^2 sr cm^{-1}) or higher than 1.25×10^{-9} W/(cm^2 sr cm^{-1})
- if there were abnormal averaging kernel values
- if the spectral fit diverged
- if the total error covariance matrix is ill conditioned;

It is also recommended to filter IASI L2 data characterized by:

- DOFS <2
- a ratio of the surface-6km column to the total column higher or equal to 0.085

Those last 2 filters have been applied to the IASI L2 data before generating the L3 datasets

3.2.3 Level 2 to Level 3

This section gives a short description of the methodology used to calculate averaged ozone fields on a regular 1°x1° latitude-longitude grid and gives a description of its output files. Input that are provided are IASI/Metop-A and IASI/Metop-B L2 satellite measurements retrieved from FORLI-O3 v20151001, output is in netcdf format. For each month, all IASI pixels falling into a grid cell are added to the corresponding grid cell. Then the average and standard deviation are calculated. The pixel values are weighted by $1/\sigma^2$ (σ being the total error associated) before adding, so the weighted mean gridcell value and the corresponding standard deviation are given by

$$mean = \frac{\sum_i \frac{x_i}{\sigma_i^2}}{\sum_i \frac{1}{\sigma_i^2}}$$

$$stddev = \sqrt{\frac{1}{\sum_i \frac{1}{\sigma_i^2}}}$$

These values are provided for total ozone column and tropospheric ozone column, for day and night time and for IASI/Metop-A and IASI/Metop-B separately in the L3 files. Day and night time data are determined with solar zenith angle to the sun <=90° and >90°, respectively. An example is illustrated in Figure 12 for January 2008, based on the L2 dataset. The current parameters included in NetCDF files are presented in Table 37 and the NetCDF files are currently available for 2008.

Figure 12 - L3 mean total ozone column (left) and its uncertainty (right) for January 2008, based on IASI/Metop-A L2 data.

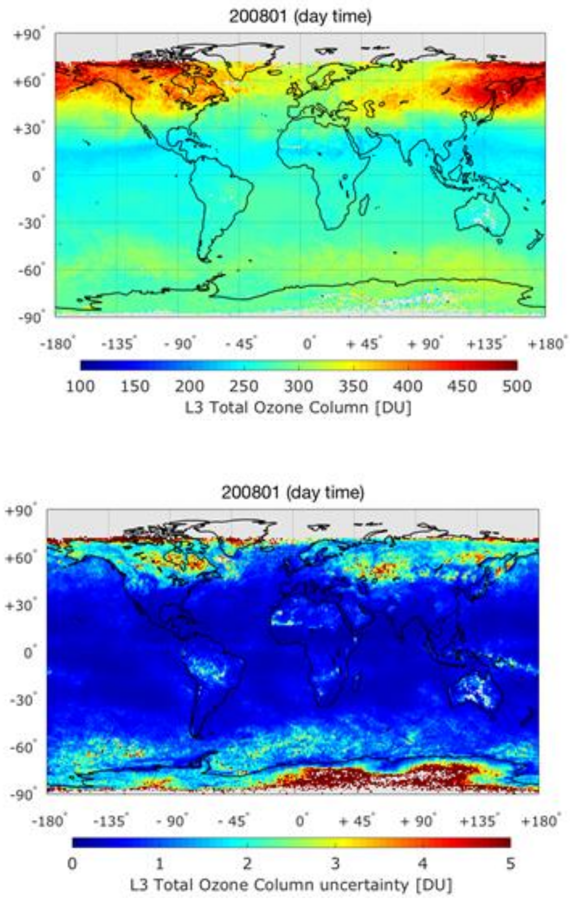


Table 37. Dimension and description of the variables contained in the current IASI-A and IASI-B L3 ozone NetCDF files. N_{lat} and N_{lon} represents the number of latitude and longitude, respectively.

Variable Name	Dimension	Unit	Description
latitude	N_{lat}	degree	latitude, from -90 (south) to +90 (north) given at gridcell centers
longitude	N_{lon}	degree	longitude, from -180 (west) to +180 (east) given at gridcell centers
total_ozone_column	N_{lat} x N_{lon}	mol m^{-2}	weighted average of the total ozone columns
total_ozone_column_error	N_{lat} x N_{lon}	mol m^{-2}	uncertainty in the weighted average of the total ozone columns
tropospheric_ozone_column	N_{lat} x N_{lon}	mol m^{-2}	weighted average of the tropospheric ozone columns
tropospheric_ozone_column_error	N_{lat} x N_{lon}	mol m^{-2}	uncertainty in the weighted average of the tropospheric ozone columns

3.3 Ozone profile retrieval from UV-nadir sensors

3.3.1 Level 1 to Level 2

3.3.1.1 Overview

The RAL nadir profile ozone scheme for the GOME-class UV sensors uses optimal estimation to directly retrieve the full vertically resolved ozone profile to ground level. Due to its sensitivity to near surface ozone, it was selected as the ESA-CCI nadir profile scheme. The RAL retrieval scheme derives profiles of number density on a set of pressure levels, spaced approximately every 4-6 km in altitude, taken from the SPARC-DI grid (*Hegglin et al., 2013*). The optimal estimation method is used. Averaging kernels are provided on this basis. It is noted that the vertical resolution of the retrieval is relatively coarse compared to the vertical grid and that tropospheric levels in particular have significant bias towards the assumed *a priori* state. It is therefore important to take account of the characterization of the retrieval provided by the averaging kernels when comparing these results to other data-sets, particularly where those are more highly vertically resolved.

Figure 13 - Retrieved number density orbit cross section on 25th August 2008 (nadir pixel).

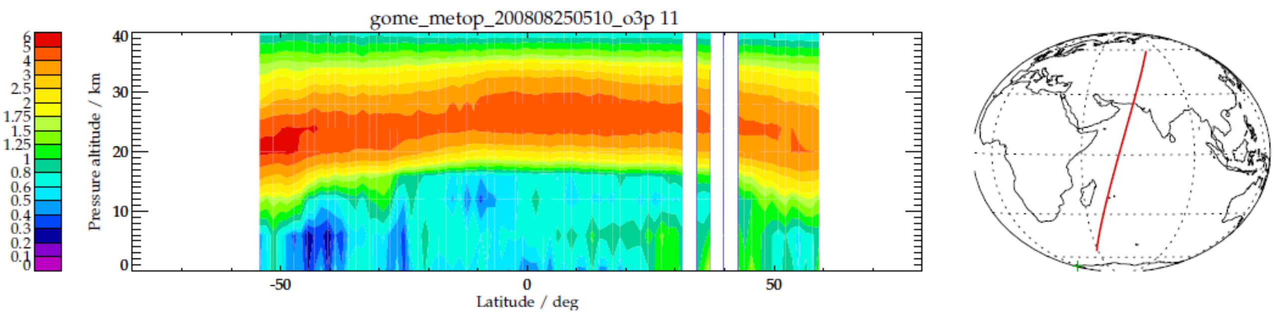
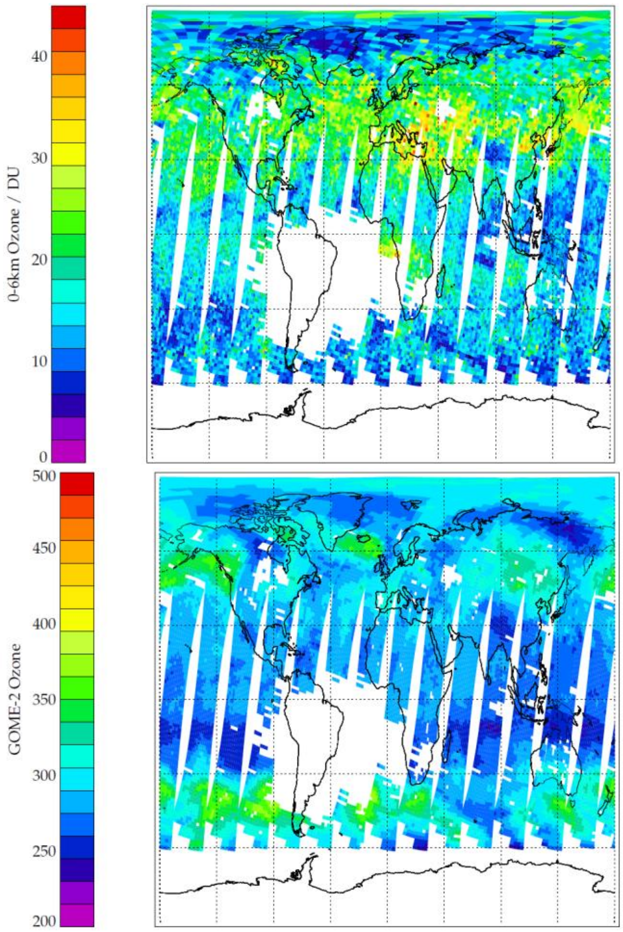


Figure 13 shows an example of retrieved number density profiles over 1 orbit. Retrieved ozone and ozone error are also provided on levels in volume mixing ratio, in addition to sub-column and sub-column error estimates. Figure 14 shows examples of the lowest retrieved sub-column and total column ozone for 1 day in August 2008. For convenience vertically integrated sub-column amounts between the retrieval levels are also reported.

Figure 14 - Lowest layer retrieved sub-column ozone on 25th August 2008 (left), and Retrieved total column ozone (right) on the same day.



The algorithm is sequential retrieval. It uses information from GOME-2 Band 1 initially before performing surface albedo retrieval in Band 2 and finally ozone profile retrieval in Band 2 incorporating the information derived from Band 1 as input. The output from both retrievals are included in the product with that from Band 1 indicated in the variable name, however it should be highlighted that the output from the Band 1 retrieval is not the algorithm final solution. Other trace gas spectra are fitted as part of the ozone retrieval in order to accurately fit the ozone profile (such as CH_2O and BrO) and their column values are included in the output file, but it should be noted that the chosen fitting window is optimized for ozone rather than these trace gases.

It is recommended that some quality control criteria be applied to the ozone profile data, using parameters also supplied within the NetCDF file:

- ‘ncost’ (the normalised total fit cost) is less than 2
- ‘aconv’ (the convergence flag) is equal to 1
- ‘sza’ (solar zenith angle) is less than 80°
- 1/cos(‘lza’)*’o3_b1_tc’ (the line-of-sight zenith component of the Band 1 retrieved total column amount) is less than 500 during the months of January to May. This is due to very high

stratospheric ozone at high Northern latitudes which limits the ability to discern tropospheric ozone beneath.

Tropospheric ozone can have a low bias in the presence of thick cloud (as indicated by ‘cloudf’ (cloud fraction) and/or high cloud ‘cloudp’ (effective cloud top pressure).

3.3.1.2 RAL Ozone Profile Algorithm Description

The RAL profile scheme (*[Munro et al., 1998], [Siddans et al., 2003], [Miles et al., 2015]*) scheme differs from the GOME-2 Operational Algorithm (www.temis.nl) in a number of important respects. The most significant difference is the treatment of the Huggins bands which are fitted to a precision of better than 0.1% (close to the noise level) to allow the ozone absorption cross-section temperature dependence to be exploited for tropospheric information. This is achieved by fitting the differential absorption spectrum (log of sun-normalised radiance with polynomial subtracted) in the Huggins range rather than the absolute sun-normalised radiance, which it is necessary to fit in the Hartley band in order to obtain information at higher altitudes. This distinct treatment of the two spectral ranges leads to the formulation of the retrieval problem in 3 steps:

1. “B1 fit”: Fit ozone profile to the sun-normalised radiance in the Harley band (in GOME Band 1) from 265-307nm.
2. “Albedo fit”: Fit effective surface albedo for the Huggins bands GOME from a narrow region (where ozone absorption is low) around 334nm (assuming the B1 ozone to be correct).
3. “B2 fit”: Add information on ozone from the differential absorption spectrum in the Huggins bands. I.e. retrieve the ozone taking the B1 result to define the prior state and errors.

Methods to improve the characterisation of sub-pixel cloud in the GOME field-of-view using Vis-near-IR imagery (ATSR and AVHRR) have been implemented in the RAL GOME scheme and can be used optionally. The potential benefit of using co-located imagery in this way to improve the O_3 ECV has been tested, providing a significant link to the cloud / aerosol ECV projects, which are planned to involve the application of the Oxford-RAL aerosol and cloud scheme to ATSR-2 and AATSR.

3.3.1.3 Basic retrieval equations

Each step of the RAL retrieval is performed using optimal estimation *[Rodgers, 2000]*. The standard equations apply.

However the linear error analysis is somewhat complicated by the 3-step retrieval approach. Particularly as the ozone prior covariance used in step 3 is not identical to the solution covariance output from step 1. This is handled by linearising each step and propagating the impact of perturbations in parameters affecting the measurements through to the final solution.

The following equations defined the averaging kernel. For the 3-step process, the averaging kernel is:

$$A = D_{y3}K_3 + D_{a3}(M_1^3 A_1 M_1^{3T} + M_2^3 A_2 M_2^{3T})$$

where the sub-scripts denote the matrices for each retrieval step and M is the matrix (consisting entirely of 0s and 1s) which maps the elements of the state vector at one step into the corresponding element of the state vector for a later step. Similarly the impact of perturbations in a forward model parameter are propagated via

$$\Delta X_b = D_{y3}\Delta b_3 + D_{a3}\left[M_1^3\left(D_{y1}\Delta b_3\right)M_1^{3T} + M_2^3\left(D_{y2}\Delta b_2\right)M_2^{3T}\right]$$

The estimated standard deviation of the final retrieval (ESD) is taken to be the square-root of the step-3 solution covariance (which includes the contribution from the other steps, in the step-3 a priori covariance).

3.3.1.4 Assumptions, grid and sequence of operations

3.3.1.4.1 Spectral ranges

In the region between 240 and 315nm there is a relatively large spectral variation in optical depth and consequent uncertainty in the fractional polarisation, which can lead to errors of the order of a few percent in sun-normalised radiance. There is a trade-off between the improvement in ESD from including as much of this range as possible and the mapping of polarisation errors (also quasi-random due to the variability of the polarisation state introduced by cloud). These errors might be mitigated by including additional retrieval parameters, but the polarisation signature is likely to correlate to the broad absorption in this range. Similarly the benefit of including channels towards the short wave end of the range is offset by increasing measurement errors, including noise and those due to imperfect modelling of dark-current and straylight. The range 265-307nm is selected as the best compromise.

From this range the following sections are ignored to avoid strong Fraunhofer lines (particularly sensitive to errors in modelled leakage current, wavelength calibration and Ring effect) and the NO gamma-bands: 265-269, 278.2-280, 284-286.4, 287.2-288.8nm.

In order to fit the Huggins bands to the required accuracy it is necessary to model the Ring effect and under-sampling. A pre-requisite of such a model is an accurate knowledge of the slit-function and the wavelength registration relative to the solar reference spectrum used in the model. For GOME-1 Pre-flight spectral calibration of the instrument was insufficient for this purpose and the scheme developed here attempts to derive the required parameters, together with a better estimate of the wavelength calibration in the region by fitting the GOME measured solar spectrum to a high-resolution solar reference spectrum.

The fitting region is restricted to 322.5 to 334nm: Below this range the fit to the solar reference spectrum shows gross changes in spectral resolution and wavelength calibration. Fit residuals are also larger.

Since B2 is primarily of interest for the relatively fine-scale temperature dependent structure, the measurements in B2 are treated in a manner analogous to DOAS. The logarithm of the sun-normalised radiance is taken and a polynomial subtracted. This removes, to a large degree, independent information on the surface reflectance which modulates the mean layer photon-path profile. It is therefore important to specify (not retrieve) an accurate surface albedo as a forward model parameter in this retrieval step. This is obtained from a separate retrieval from measurements in the Huggins absorption minima between 335-340nm. It is assumed that this range is close enough in wavelength to the B2 range used for the retrieval and that the albedo is appropriate, while being sufficiently insensitive to absorption, so that the B1 fitted profile can be assumed for the Huggins band albedo fit.

After restricting the spectral range and adopting the quasi-DOAS approach above, systematic residuals remained at the 0.2% level (in sun-normalised radiance). For GOME-1 and SCIAMACHY, the mean residual over a single orbit was determined. The retrieval and FM were then modified to allow this pattern to be added to simulated measurements, scaled by a retrieved parameter. For GOME-2 a similar approach is applied, but this is currently being refined to further improve the fit.

The B1 and B2 retrievals both make use of the estimated random error on measurements provided by appropriate photon noise model. In both cases, the matrix is assumed diagonal. However, in both steps noise-floors (upper limits on the fitting precision) are imposed. The noise-floor values are arrived at empirically by inspection of fitting residuals and comparison of retrievals with climatology and validation data. In B1 the noise floor is set to 1% in sun-normalised radiance unit. In B2 the value varies with solar zenith angle, but is typically 0.05% (0.0005 in units of the natural log of the sun-normalised radiance).

Since the absolute sun-normalised radiance is used in the B1 fit, and this is subject to degradation over time (which varies from instrument to instrument), an empirical correction scheme is used to correct the L1 data in the B1 range used. This is based on modelling observed radiances based on climatological ozone distributions and fitting a polynomial in time (sufficient to capture seasonal variations) and wavelength (4th order over the band) which captures the deviations of the observations from the climatological predictions.

3.3.1.4.2 Vertical grid

Vertical grids are defined for the retrieval state vector and for the RTM finite-difference computational levels. To minimise changes in the scheme as it is applied globally, the same sets of levels are always used. The levels are defined in terms of pressure, so as to follow the meridional variation in tropopause height more closely than geometric altitude. They are referred to in terms of a scale-height in km, referred to as Z^*:

$$Z^*/\mathrm{km} = 16[3.0 - log_{10}(p/\mathrm{hPa})]$$

where p is pressure in hPa. This gives a value comparable to geometric height (within about 1km).

3.3.1.4.3 Ozone state vector

The state vector elements for ozone are the logarithm of the volume mixing ratio. Retrieval levels are defined to be 0, 6, 12 km, then at 4 km intervals up to 80 km (corresponding always to the same pressure levels of approximately 1000, 422, 177, 100.000, 56, 32, 18, 105.6, 3.2, 1.8, 1.0, 0.56, 0.32, 0.18, 0.10, 0.056, 0.032, 0.018, 0.01 hPa). These over-sample the resolution expected on the basis of averaging kernel analysis. The *a priori* covariance is used to constrain the profile shape.

An *a priori* correlation length of $\Delta z_c = 6\mathrm{km}$ is imposed for the Hartley band fit (Step 1), i.e. the elements of $S_a$are given by

$$(S_a)_{ij} = \Delta x_{ai}\Delta x_{aj}e^{-\left(\frac{z_j - z_i}{\Delta z_c}\right)^2}$$

The values of the *a priori* and corresponding errors, Δx_{aj}, at each level i, at altitude z_j, are taken from the *McPeters-Labow* (*McPeters et al., 2007*) or *Fortuin* (*Fortuin and Langematz, 1994*) climatology interpolated in altitude to the retrieval grid.

For the B2 fit, the *a priori* is taken from the B1A retrieval, on the same levels. Instability in the retrieval at UT/LS altitudes was encountered when the full solution covariance, from the B1A retrieval was taken to define for the B2B retrieval. This instability was reduced by using a Gaussian *a priori* covariance with 8km correlation length and *a priori* standard deviation equal to B1A ESD.

The following deviations from the *Fortuin* climatology are imposed:

- At the surface and 6 km levels, the volume mixing ratio is set to the larger of the climatological value and a value corresponding to a number density of 10^{12} molec/cm^3. In practice, both levels are always set to this value except at very high latitude where the climatological value is greater on the 6km level. I.e. there is no horizontal structure in the *a priori* at these levels. This approach is intended to minimise the appearance of spurious spatial/temporal patterns in retrievals at tropospheric altitudes due to *a priori* influence.
- To avoid too tight an *a priori* constraint, and to avoid spurious effects in the retrieval due to the imperfect sampling of the tropospheric variance by the climatology, the relative *a priori* errors were set to the larger of the climatological standard deviation and the following:
    - 0-12km: 1 (in logarithmic units corresponding to 100% in fractional terms).
    - 6km: 0.3
    - 20-50km: 0.1
    - 56km: 0.5
    - 60-80km: 1

3.3.1.4.4 Other state vector elements: B1 fit

Leakage Current: A leakage current in binary units is fitted in B1, to correct for imperfect prediction of this at L1. A single parameter is fitted for the band, unless the B1A/B1B boundary occurs below 307nm, in which case one parameter is fitted for each sub-band. The leakage current in BU is assumed constant with wavelength.

Lambertian effective surface albedo: A single, wavelength independent albedo is retrieved.

Ring effect: Two parameters are fitted, namely (i): Scaling factor for the single-scattering Ring effect filling-in factor (as modelled via the approach of *[Joiner et al., 1995]*; (ii) Wavelength shift of the pattern relative to the nominal wavelength calibration.

Wavelength shift of the absorption cross-section: A single parameter represents a shift of the GOMETRAN modelled spectrum (before Ring effect or slit-function convolution are simulated), with respect to the measured sun-normalised radiance. The magnitude of the retrieved shift is such that it can be considered to pertain effectively to the trace-gas absorption cross sections, since the scattering coefficient varies relatively weakly with wavelength.

3.3.1.4.5 Other state vector elements: B2 fit

Ring effect: A single scaling parameter is fitted (to represent approximately the expected number of scattering events). No wavelength shift is fitted in this case; the mis-registration / under-sampling correction makes the shift of the filling-in spectrum redundant.

Wavelength shift of the absorption cross-section: The parameter has the same meaning as the corresponding B1A state-vector element. In this case a 2nd order polynomial fit to the wavelength shift is fitted across the measurement vector range.

Wavelength mis-registration between solar and back-scattered spectrum: Parameters in 3rd order polynomial expansion (as above) of the wavelength shift between the GOME solar irradiance and back-scattered spectra used to form the sun-normalised radiance.

Column amounts of **NO_2, formaldehyde** and **BrO**.

Residual scaling factor: A single scaling factor for the systematic residual.

3.3.1.5 Iterations and convergence

The standard Marquardt-Levenberg approach is used. Convergence is judged to occur if (a) the cost function (absolute value, not normalised by the number of elements in the state vector) changes by <1 (b) at this point a Newtonian iteration (i.e. a step without applying the Marquardt-Levenberg damping) also results in a change in cost of <1. This 2nd criterion ensures retrievals do not appear to converge due to a high value of the Marquardt-Levenberg damping parameter.

3.3.1.6 Forward model

3.3.1.6.1 Atmospheric state input to the RTM

Temperature and pressure profiles are taken from meteorological analysis. Usually ECMWF profiles are used, though Met Office stratospheric analysis have been used in the past.

A background aerosol profile taken from MODTRAN is assumed.

Cloud may be ignored (in which case it is fitted via the retrieved surface albedos) or modelled according to information either from GOME (O_2 A-band retrieval) or co-located imagery (AATSR for GOME-1 and AVHRR for GOME-2).

3.3.1.6.2 Radiative Transfer Model (RTM)

The scheme uses a version of the GOMETRAN++ *[Rozanov et al., 1997]* but with a number of processing speed improvements implemented at RAL.

3.3.1.7 Error description

A quite complete study of the errors pertaining to the profile retrieval is reported in *[Siddans, 2003]*. This was based on performing retrieval simulations for a set of basic geo-physical scenario which had been defined for the GOME-2 Error Study *[Kerridge et al., 2002]* (which also contains a detailed error budget). For these conditions basic retrieval diagnostics such as averaging kernels (e.g. see Figure 15) and solution covariances were computed. A large number of additional error sources were also considered.

Figure 16 shows some results from *[Siddans 2003]*. The following errors are considered

- Aerosol: Errors in retrieved ozone introduced by deviations in the aerosol profile from the background case assumed in the FM are simulated by mapping measurement perturbations based on the following cases: [HIGH] represents a maximum boundary layer / troposphere optical depth case from the MODTRAN scenarios, with a moderate volcanic stratosphere. [BL10], [SUM] and

[MODVOL] are close to the background case except in the boundary layer, troposphere and stratosphere respectively, where they are close to the [HIGH] scenario.
- [PRESSURE]: Effect of a 1% perturbation in surface pressure on scattering profile and hence retrieval (absorber number density not perturbed).
- [TEMP-2KM]: Effect of 1K error in assumed temperature profile on 2km grid. Both temperature errors are propagated through the absorption cross-section only (i.e. not via number density profile).
- [TEMP-10KM]: As, above but assuming a Gaussian correlation with 10km half-width. [TEMP-FCBKG]: As above, but taking the covariance matrix from a numerical weather prediction background error covariance matrix.
- [TEMP-IASI] As [TEMP-FCBKG], but using the estimated covariance after assimilation of IASI information.
- [MIRROR]: Errors due to the incidence angle dependence of the scan-mirror degradation.
- [POLERR-G1]: Estimated effect of error in polarisation correction given GOME-1 correction scheme (and PMD data).
- [RADCAL]: 2% Gain error. I.e. mapping of a 2% of the nominal back-scattered radiance is mapped as a systematic error, to represent radiometric calibration errors.

The most important findings of the error assessment described here are summarised as follows:

- The retrieval provides useful information on the ozone profile below 50km.
- Retrieval precision, accounting for measurement noise and other quasi-random errors is expected to be generally in the few-percent range in the stratosphere increasing to a few 10s of percent in the lowest retrieval levels.
- Retrieved quantities should be interpreted as estimates of layer-averaged number density, taking into account the shape of the averaging kernels, and the influence of the a priori.
- The instrumental and RTM errors are generally relatively small, compared to the climatological variance and, in most cases, the ESD. Exceptions are radiometric gain errors including scan-mirror degradation (which has most impact above 40km) and possibly imperfect knowledge of slit-function shape (expected to cause a significant negative bias in the troposphere, though the magnitude is difficult to quantify). These errors are currently addressed in the real scheme by the empirical degradation correction factor, but still represent a significant issue for long-term quality of the retrieved profiles.
- High perturbations in aerosol and errors in the assumed temperature profile give rise to retrieval errors in the troposphere of order 10-20%. (The temperature error is larger at high solar zenith angle.)
- Radiative transfer model approximations in the retrieval scheme are seen to be adequate.
- It was also noted that for GOME-1 a significant error source was lack of pre-flight measurement of the slit-function. Pre-flight characterisation of GOME-2 has much reduced uncertainties for that instrument at the beginning of life but in-orbit changes may mean this source of error is important for GOME-2 as well.

3.3.1.8 Output product description

Retrieval results are output in ncdf format following CF convertions. See the Product User Guide for details. The product contains the retrieved profile (values on the retrieval levels), partial columns (integrated between retrieval levels), the full error covariance matrix, the retrieval noise covariance matrix, the a-priori profile the averaging kernels and the retrieved auxiliary parameters. Also included are: geolocation, spectral windows used and retrieval diagnostics, like number of iterations, spectral fit indicators. Each file contains results for a single orbit.

Figure 15 - Averaging kernels (in units of retrieved number density / unit perturbation to true number density) for a range of geophysical conditions typical of given months (top to bottom) and latitudes (left to right). From *[Siddans, 2003].*

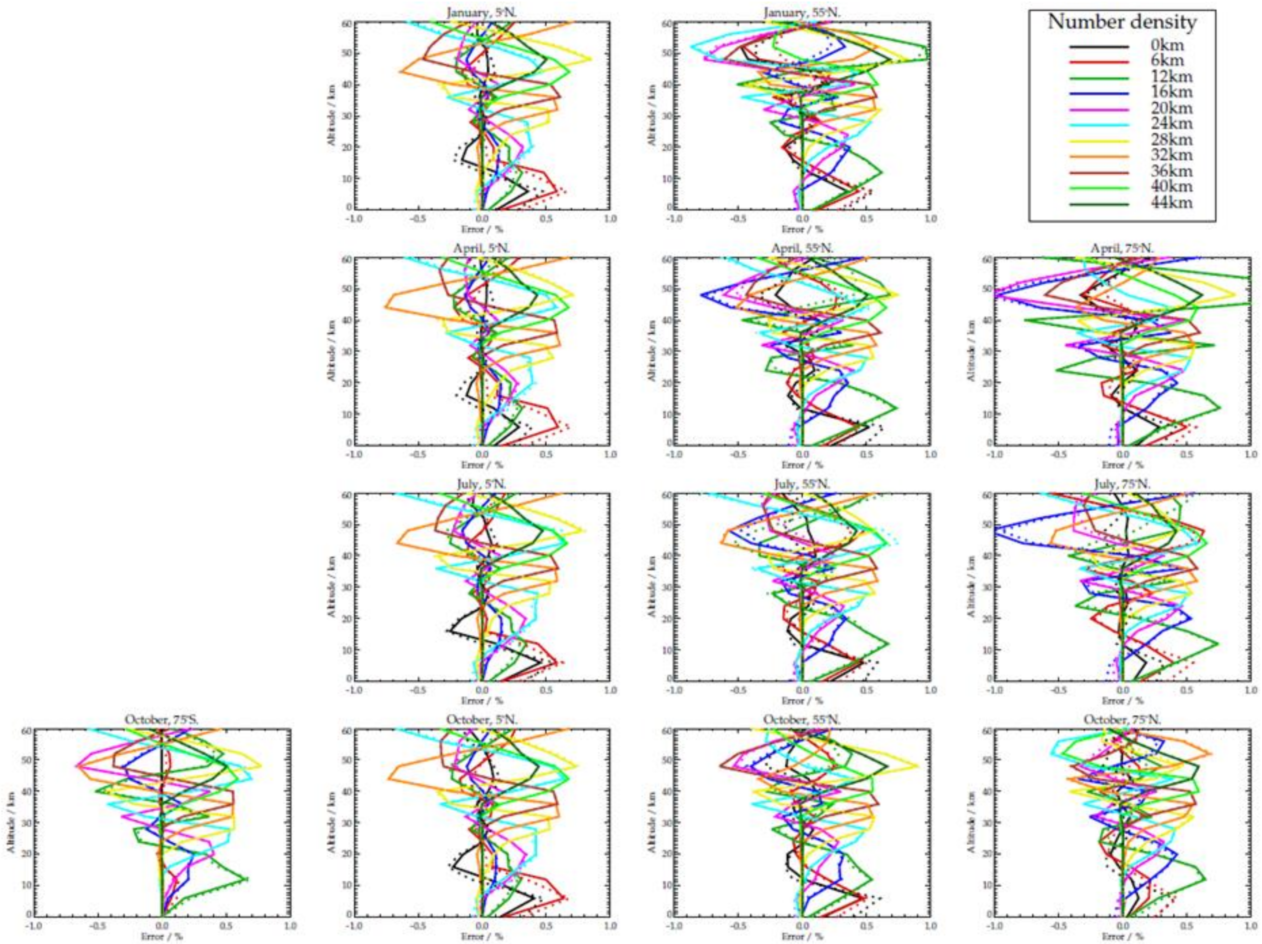
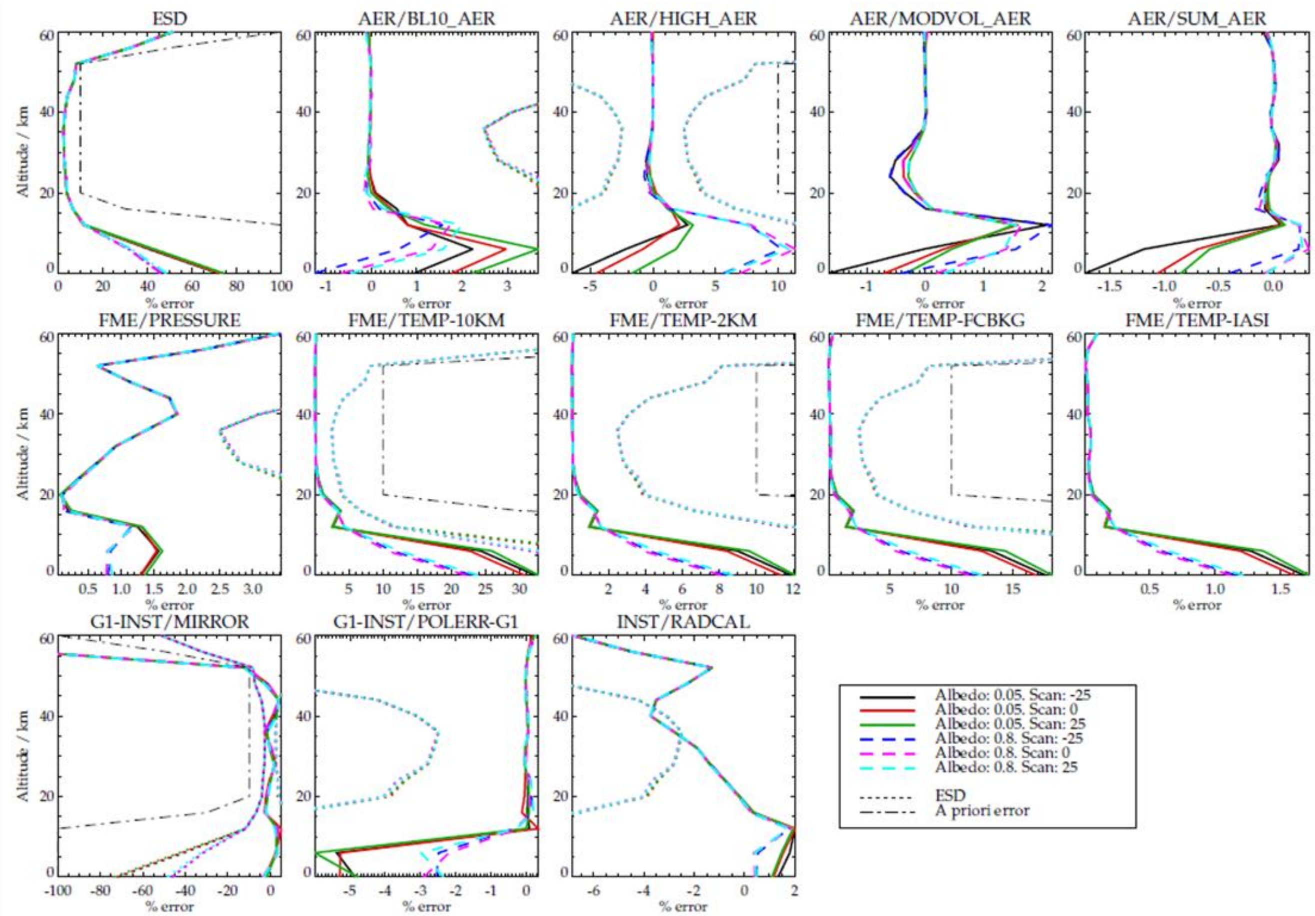


Figure 16 - Retrieval ESD and base-line mapped errors for GOME-1 and the April 55°N scenario.

Dashed and solid lines refer to the 80% and 5% surface albedo cases respectively. Colours distinguish results for the 3 across-track ground pixels in B1 (the legend shows the pixel mean off-nadir angle in degrees; positive angle are East of nadir). Dotted lines in each panel other than the top left show (for comparison) the ESD where the scale permits. The black dash-dot curve is the a priori error input to the B1 retrieval. (ESD and a priori are also plotted as negative values for comparison with negative mapped errors.)

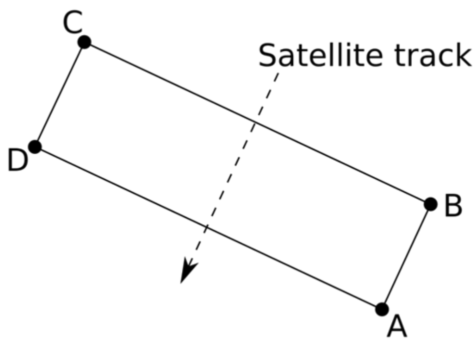


3.3.2 Level 2 to Level 3 - From satellite track to regular longitude-latitude grid

This section gives a short description of the algorithm that calculates averaged ozone fields on a regular latitude-longitude grid and gives a description of its output files. Input that should be provided are L2 satellite measurements, output is in NetCDF format complying with the CF 1.6 metadata conventions.

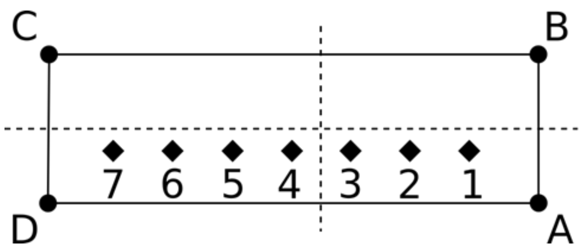
The pixels in the satellite data (L2) are assumed to be ordered as indicated in Figure 17. If this is not the case, the reading routine should provide the appropriate transformation. **A** is the first corner in the longitude and latitude arrays, **B** the second etc. The across track direction is given by the lines the lines **A**-**D** and **B**-**C**, while the along track direction is given by the lines **A**-**B** and **D**-**C**. Note that corners **C** and **D** are reversed with respect to the GOME/GOME-2 convention.

Figure 17 - Pixel layout assumed in the nadir L3 algorithm.



The along track pixel edges **AB** and **DC** and cross track pixel edges **AD** and **BC** (see Figure 17) are divided into a number of points. The first point on **AB** and the first on **DC** form a line which is divided into the same number of points as **AD**. Each of these points is assigned to a gridcell, see for example Figure 18.

Figure 18 - A L2 pixel is divided into subpixels (diamonds 1-7). Each subpixel is assigned to a TM5 gridcell (dashed) and the average and standard deviation are calculated (see text).



Suppose that ABCD in Figure 18 is the pixel of interest and that the horizontal line marked with the diamonds are the subpixels (numbered 1 to 7). Furthermore, the two dashed lines denote the gridcell boundaries which are numbered the same way as the pixel corners (i.e. gridcell A is the lower right cell). In this case, subpixels 1 ∼ 3 are added to gridcell A, and the counter for gridcell A is increased by 3. Subpixels $4 \sim 7$ are added to gridcell D and the counter for gridcell D is increased by 4. The pixel values are weighted by $1/\sigma^2$ before adding, so the weighted mean gridcell value and the corresponding standard deviation are given by:

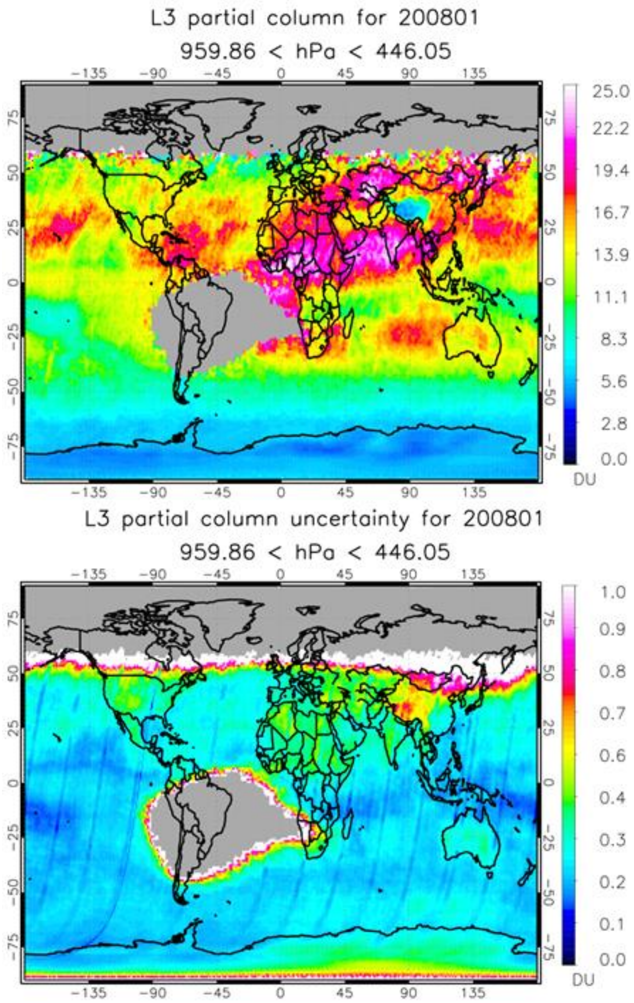
$$mean = \frac{\sum_i \frac{x_i}{\sigma_i^2}}{\sum_i \frac{1}{\sigma_i^2}} \qquad \text{Eq. (25)}$$

and

$$sdev = \sqrt{\frac{1}{\sum_i \frac{1}{\sigma_i^2}}} \qquad \text{Eq. (26)}$$

These values are provided for partial columns in the L3 files on a layer-by-layer basis and for the total column. An example is shown in Figure 19 for January 2008, based on the L2 dataset provided in Phase 1 of the ozone CCI project.

Figure 19 - Mean partial ozone column (left) and its uncertainty (right) for January 2008, based on L2 data provided in the first phase of the Ozone-CCI project.



3.4 Ozone profile retrieval from limb and occultation sensors

3.4.1 Heritage

Algorithms applied to the retrieval of Level-2 ozone profiles from Level-1 data collected by limb and occultation sensors are described in the Ozone_CCI ATBD *[RD-22]*. In the Ozone_CCI project, the L-2 ozone profiles are harmonized and serve as input to the generation of Level-3 ozone profiles. The same approach is used in the C3S Ozone project.

3.4.2 Harmonisation of Level 2 profiles

The HARMonized dataset of OZone profiles (HARMOZ) is based on limb and occultation measurements from Envisat (GOMOS, MIPAS and SCIAMACHY), Odin (OSIRIS, SMR) and SCISAT (ACE-FTS) satellite instruments *(Sofieva et al., 2013)*. HARMOZ consists of original retrieved ozone profiles from each instrument, which are screened for invalid data by the instrument teams. While the original ozone profiles are presented in different units and on different vertical grids, the harmonized dataset is given on a common pressure grid in NetCDF-4 format. In its original version, HARMOZ used a pressure grid as a vertical coordinate. The Ozone_cci pressure grid corresponds to vertical sampling of ~1 km below 20 km and 2-3 km above 20 km. The vertical range of the ozone profiles is specific for each instrument, thus all information contained in the original data is preserved, provided altitude and temperature profiles allow the representation of ozone profiles in number density or mixing ratio on a pressure or altitude vertical grids. Geolocation, uncertainty estimates and vertical resolution are provided for each profile. For each instrument, optional parameters, which are related to the data quality, are also included.

The detailed description of the HARMOZ data can be found in *Sofieva et al., 2013*. The dataset is available at [http://www.esa-ozone-cci.org/?q=node/161 or at dx.doi.org/10.5270/esa-ozone_cci-limb_occultation_profiles-2001_2012-v_1-201308](http://www.esa-ozone-cci.org/?q=node/161).

For climate studies, it is preferable to use only the information provided in the dataset (and avoid as much as possible using the data from models and reanalyses). Furthermore, as shown by McLinden and Fioletov *(McLinden and Fioletov, 2011)*, ozone trends inferred from number density on altitude grid measurements are different from those in mixing ratio on pressure grid due to temperature changes in the atmosphere. This difference is more pronounced at upper altitudes. Therefore, the original HARMOZ dataset was updated with the new data versions and called hereafter as HARMOZ_PRS, while HARMOZ_ALT is the harmonized dataset of altitude-gridded number density ozone profile. In HARMOZ_ALT, the vertical grid is with 1 km spacing (every integer kilometer). We would like to note that the number density on altitude grid is the “native” representation for the instruments included into the merged ozone dataset (see Section 3.4.3.2 below for more details).

3.4.3 Level 2 to Level 3

For creation of Level 3 data sets, the harmonized Level 2 ozone profiles from the limb/occultation sensors of the Ozone_cci data base are used.

3.4.3.1 Level 3 ozone profiles from individual limb and occultation sensors

The monthly zonal mean data in 10° latitude zones from 90°S to 90°N are created for all Ozone_cci limb and occultation instruments. The most recent versions of HARMOZ data are used as an input.

For all sensors, the monthly zonal average is computed as the mean of ozone profiles. x_k :

$$\rho = \frac{1}{N}\sum x_k \qquad \text{Eq. (27)}$$

where *N* is the number of measurements, $N > 10$. The mean estimate has been chosen in order to minimize artificial biases, which might appear when using weighted mean or median estimates. The uncertainty of the monthly mean σ_ρ^2 is estimated as the standard error of the mean:

$$\sigma_\rho^2 = \frac{s^2}{N} \qquad \text{Eq. (28)}$$

where $s^2 = \langle (x_k - \bar{x})^2 \rangle$ is the sample variance. For the sample variance, we used its robust estimate as $s = 0.5 \,.\, (P_{84} - P_{16})$, where P_{84} and P_{16} are 84th and 16th percentiles of the distribution, respectively. An example of monthly zonal mean, standard deviation and standard error of the mean at 15-50 km for January 2008, for the Ozone_cci instruments is shown in Figure 20. As observed fromFigure 20, the ozone distributions are very similar in the datasets. Due to large number of averaged data, the standard error of the mean is usually less than 1% in the stratosphere.

Both sample standard deviation *s* and the standard error of the mean σ_ρ are stored in the MZM files.

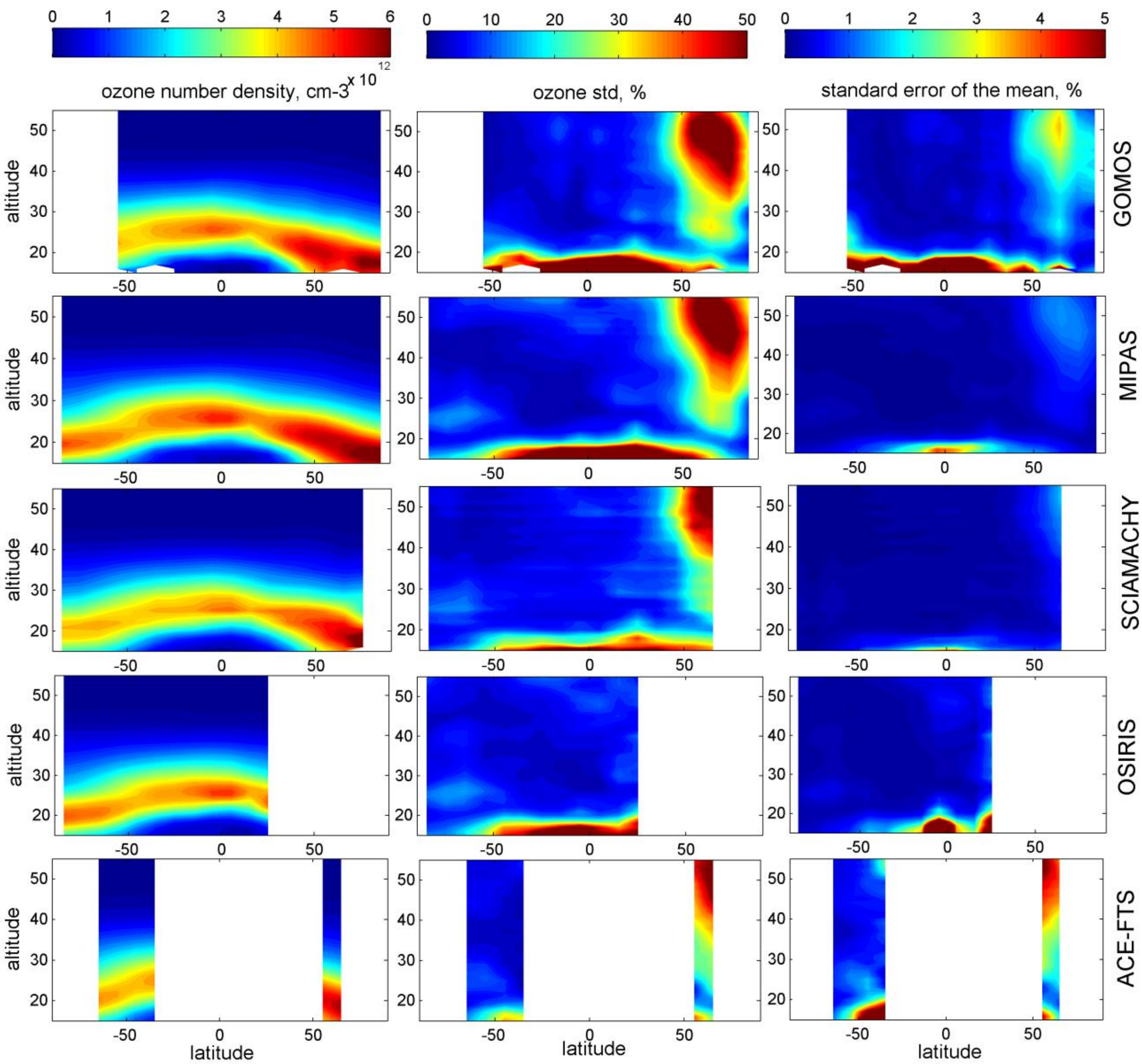
The mean of individual error estimates e_k :

$$\bar{e} = \frac{1}{N} \sum e_k \qquad \text{Eq. (29)}$$

is also provided in the MZM data files.

In order to characterize the non-uniformity of sampling, we provide inhomogeneity measures in latitude, H_{lat}, and in time, H_{time}. The definition of this measures and details of the related analyses can be found in *(Sofieva et al., 2014)*. Each inhomogeneity measure ranges from 0 to 1 (the more homogeneous, the smaller *H*). For dense samplers (MIPAS, SCIAMACHY, OMPS), the inhomogeneity is close to zero nearly for all latitude bins. For other instruments, inhomogeneity measure can be large for some latitude-time bins.

Figure 20 - Left: monthly zonal mean ozone profiles for January 2008 for Ozone_cci instruments, center: standard deviation of ozone profiles in %, right: standard error of the mean, Eq. (28).



3.4.3.2 Merged monthly zonal mean (MMZM) ozone profiles

3.4.3.2.1 Overview

For the merged dataset, all reliable satellite data, which provide ozone profiles on altitude grid, are used. The merged dataset is targeted to serve as a climate data record for assessment of ozone trends. The data from five Ozone_cci instruments: GOMOS, MIPAS, SCIAMACHY, OSIRIS and ACE-FTS covering the period 2001- present (Envisat data are in the period of 2002-2012), are merged with the data from SAGE II (1984-2005) and OMPS (2002- present). Hereafter, we will refer to this dataset as SAGE II-CCI-OMPS, for short.

The stability of the individual-instrument data records has been extensively studied; only stable data are used for the merged dataset. The merging is performed on the deseasonalized anomalies computed from each individual dataset. This method is often exploited for creating a long-term data record and for trend analysis.

All the data used for creating the merged dataset have a sufficiently good resolution of 2–3 km in the UTLS. For all instruments, ozone profiles are retrieved on the geometric altitude grid. The majority of the datasets -SAGE II, GOMOS, OSIRIS, SCIAMACHY and OMPS - provide number density ozone profiles; therefore this representation is used for the merged dataset. For ACE-FTS and MIPAS, the retrievals are in volume mixing ratio on altitude grid. Conversion to number density profiles is performed using temperature profiles retrieved by these instruments, thus providing consistent (i.e., without using external information about temperature and pressure profiles) representation of number density ozone profiles.

The information about individual datasets is collected in Table 38. For some instruments, the selected time period is shorter than the full operation period. The individual datasets have been compared with each other and with ground-based data, and only the time periods when the instruments were operating the best are selected.

Table 38. Information about the datasets used in the merged dataset (ozone profiles from limb and occultation sensors).

Instrument/ satellite	Processor, data source	Time period	Local time	Vertical resolution	Estimated precision	Profiles per day
SAGE II/ ERBS	NASA V7.0, original files	Oct 1984 – Aug 2005	sunrise, sunset	~1-2 km	0.5-5%	14-30
OSIRIS/ Odin	USask v 5.10, HARMOZ_ALT	Nov 2011 – present	6 a.m., 6 p.m.	2-3 km	2-10%	~250
GOMOS/ Envisat	ALGOM2s v 1.0, HARMOZ_ALT	Aug 2002 – Aug 2011	10 p.m.	2-3 km	0.5–5 %	~110
MIPAS/ Envisat	KIT/IAA v.7, HARMOZ_ALT	Jan 2005 – Apr 2012	10 p.m., 10 a.m.	3-5 km	1–4%	~1000
SCIAMACHY/ Envisat	UBr v3.5, HARMOZ_ALT	Aug 2003- Mar 2012	10 a.m.	3-4 km	1-7%	~1300
ACE-FTS/ SCISAT	V3.5/3.6, HARMOZ_ALT	Feb 2004 – present	sunrise, sunset	~3 km	1-3%	14-30
OMPS/ Suomi NPP	USask 2D, HARMOZ_ALT	Apr 2012- present	1:30 p.m.	~2 km	2-10%	~1600

The merged dataset is created in 10° latitude zones from 90°S to 90°N, in the altitude range 10 – 50 km.

3.4.3.2.2 Merging method. Merged deseasonalized anomalies

The merging is performed through computation of normalized deseasonalized anomalies from individual instruments and merging them. For each instrument, latitude zone and altitude level, the deseasonalized anomalies are computed as:

$$\Delta(t_i) = \frac{\rho(t_i) - \rho(m)}{\rho(m)} \qquad \text{Eq. (30)}$$

where $\rho(t_i)$ is monthly zonal mean value at certain altitude and latitude zone corresponding to time t_i and $\rho(m)$ is the mean value for the corresponding month, i.e. $\rho(m) = \frac{1}{N_m}\sum_{j=1}^{N_m} \rho_j$, where N_m is number of monthly mean values ρ_j for month m.

For the Ozone_cci instruments, the seasonal cycle is evaluated using the overlapping period, years 2005-2011. The seasonal cycle for SAGE II is computed using years 1985-2004, and for OMPS using the years 2012-2016. In computation of deseasonalized anomalies, we ignore those latitude-time bins with the mean inhomogeneity $H_{tot} = 0.5(H_{lat} + H_{time}) > 0.8$.

After the removal of seasonal cycle, the SAGE II anomalies are offset to the mean Ozone_cci anomalies in years 2002-2005. The OMPS deseasonalized anomalies are offset to the mean Ozone_cci anomalies (which are based on OSIRIS and ACE-FTS measurements in this period) in years 2012-2016.

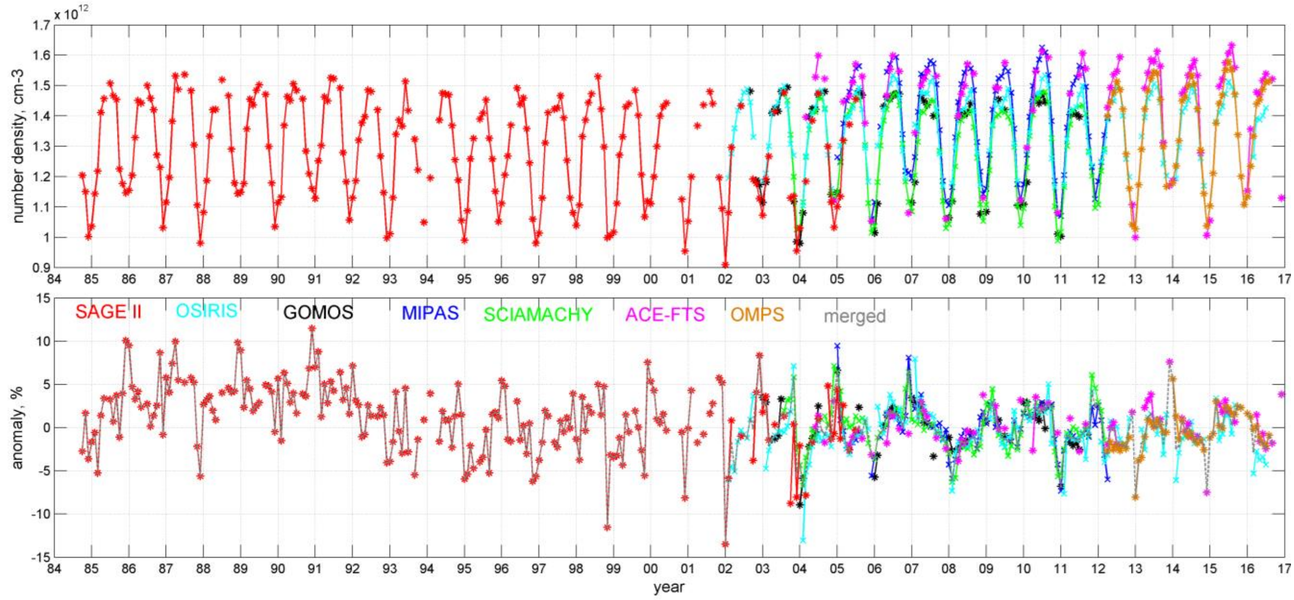
Before merging, the deseasonalized anomalies of the individual instruments have been extensively inter-compared with each other by computing and visualizing the time series of difference of individual anomalies from the median anomaly. This method turns out to be a sensitive method for detecting a temporal exceptional behavior of the individual data records. Only reliable datasets, which agree with each other and have no evident drifts or exceptional features with respect to the median anomaly, are selected for the merged dataset.

We computed the merged anomaly as the median anomaly of the anomalies from individual instruments, for each altitude level and for each latitude zone. Figure 21 illustrates the data merging: the upper panel shows the monthly zonal mean data, while the bottom panel shows individual anomalies and the merged (median) anomaly.

As observed in Figure 21, the biases between the individual data records are removed by computing the deseasonalized anomalies. In the merging, we filtered individual anomaly values (locally for each latitude zone and altitude level), which differ from the median anomaly more than 10% at latitudes 40S-40N, and more than 20% in other latitude zones. This filtering is ineffective in absolute majority of cases; it removes only a few exceptional anomalies from GOMOS and ACE-FTS data due to their insufficient sampling.

More examples of merged deseasonalized anomalies are shown in *(Sofieva et al., 2017b)*. Since absolute values are not important for trend analyses, the merged deseasonalized anomalies can be directly used in time series analyses. The evaluation of ozone trends using the merged SAGE II-CCI-OMPS has been performed in *(Sofieva et al., 2017b)* and *(Steinbrecht et al., 2017)*. The ozone trends are in agreement with those obtained using other datasets, and they are similar to that reported in *(WMO, 2014)*: strong negative ozone in the upper stratosphere before 1997 are transformed into positive.

Figure 21 - Top: monthly zonal mean ozone at 35 km in the latitude zone 40-50N. Bottom: individual deseasonalized anomalies and the merged anomaly (grey).



3.4.3.2.3 Merged ozone profiles. Notes related to the data usage.

The main dataset consists of the merged deseasonalized anomalies and their uncertainties described above. For the purpose of other applications (e.g., comparisons with models etc.), we presented the ozone profile also in number density. The computing of merged number density profiles from the merged deseasonalized anomalies is performed according to Eq. (30): the seasonal cycle is restored in the data. The best estimate of the amplitude of seasonal cycle is given by MIPAS measurements, because they provide all season pole-to-pole measurements with dense sampling. We take the absolute values of the seasonal cycle from SAGE II and OSIRIS in the overlapping period (which are very close to each other and also with GOMOS measurements), thus preserving the consistency in the dataset through the whole observation period.

For trend analyses, it is recommended using the deseasonalized anomalies directly. According to the merging principle, the best quality of the merged dataset is in the stratosphere in the latitude zone from 60°S to 60°N. The data in polar regions are affected by large variability and non-uniform data coverage. The quality of the data in polar regions is under investigation.

The satellite data quality also degrades in the UTLS. The merging principle seems to be optimal also for the UTLS, as it removed automatically biases, which can be significant in the UTLS. The trends in the UTLS estimated using the merged SAGE II – CCI- OMPS data follow the expectations (declining ozone trends in the tropics just above the tropopause due to intensification of the Brewer-Dobson circulation).

3.4.3.3 Merged monthly mean gridded ozone profiles

The monthly zonal mean gridded ozone profile dataset is provided in the altitude range from 10 km to 50 km. It covers the time period from late 2001 until now. The data are gridded monthly in the 10° latitude x 20° longitude zones. Since the sampling of solar occultation measurements is rather low, they are not included. The gridded ozone profiles are presented for GOMOS, MIPAS, SCIAMACHY and OSIRIS are first computed separately and then merged into one dataset. The information about the individual datasets can be found in Table 38. The principle of creating the Level 3 gridded data for individual datasets, as well as data merging is the same as for the monthly zonal mean dataset (see Section 3.4.3.2).

4. Output data

A basic description of the C3S ozone output fields is provided in this Section. For further detail, please see the C3S Ozone Product User Guide and Specification *[RD-24]*.

4.1 Overview

All C3S ozone data sets

- are Level-3 or Level 4 data, i.e. are provided on a regular longitude-latitude grid (or latitude bands for zonal averages);
- cover the globe;
- are monthly averages;
- are provided in CF-compliant NetCDF format.

The list of all C3S_312b_Lot2 data products is provided in Table 39.

Table 39. List of the C3S ozone data products available from the C3S CDS (March 2021). All products cover the globe and have a monthly temporal resolution. Data are provided in the NetCDF format.

Product name	Product definition	Sensor(s)	Processing level	Product type	Overall temporal coverage	Update frequency	Spatial resolution	Uncertainty information	Provision & provenance
TC_GOME	Total ozone column	GOME	3	CDR	06.1995 - 07.2011	N/A	1°x1°	Random and smoothing error	BIRA/DLR
TC_SCIA		SCIAMACHY	3	CDR	08.2002 - 04.2012	N/A	1°x1°		BIRA/DLR
TC_GOME2A		GOME-2A	3	ICDR	01.2007 - 10.2020	Quarterly with 4 months delay	1°x1°		BIRA/DLR
TC_GOME2B		GOME-2B	3	ICDR	01.2013 - 10.2020		1°x1°		BIRA/DLR
TC_OMI		OMI	3	ICDR	10.2004 - 10.2020		1°x1°		BIRA/DLR
TC_OMPS		OMPS-NM	3	ICDR	01.2012 - 10.2020		1°x1°		BIRA/DLR
TC_GTO-ECV		GOME, SCIA, GOME-2A/B, OMI	3	ICDR	07.1995 - 10.2020	Semi-annually with 4 months delay	1°x1°	Random and sampling error	BIRA/DLR
TC_MSR		(1)	4	ICDR	04.1970 - 12.2020	Annually with 3 months delay	1°x1°	Forecast error cov.	KNMI
TC_IASI-A	Total and tropospheric ozone	IASI-A	3	ICDR	10.2007 - 01.2021	Quarterly with 1 month delay	1°x1°	Random error	LATMOS
TC_IASI-B		IASI-B	3	ICDR	05.2013 - 01.2021		1°x1°	Random error	LATMOS
06TC_IASI-A		IASI-A	3	ICDR	10.2007 - 01.2021		1°x1°	Random error	LATMOS
06TC_IASI-B		IASI-B	3	ICDR	05.2013 - 01.2021		1°x1°	Random error	LATMOS
NP_GOME	Ozone profile (nadir)	GOME	3	CDR	06.1995 - 06.2011	N/A	1°x1°	Random and smoothing error	RAL/KNMI
NP_SCIA		SCIAMACHY	3	CDR	08.2002 - 04.2012	N/A	1°x1°		RAL/KNMI
NP_GOME2A		GOME-2A	3	ICDR	01.2007 - 10.2020	Annually with 4 months delay	1°x1°		RAL/KNMI
NP_GOME2B		GOME-2B	3	ICDR	04.2013 - 12.2017		1°x1°		RAL/KNMI
NP_OMI		OMI	3	ICDR	10.2004 - 10.2020		1°x1°		RAL/KNMI
LMZ_MIPAS	Ozone profile (limb)	MIPAS	3	CDR	07.2002 - 04.2012	N/A	10° lat zones	Random and sampling error	UNI-HB/FMI
LMZ_GOMOS		GOMOS	3	CDR	08.2002 - 12.2011	N/A	10° lat zones		UNI-HB/FMI
LMZ_SCIA		SCIAMACHY	3	CDR	08.2002 - 03.2012	N/A	10° lat zones		UNI-HB/FMI
LMZ_SAGE2		SAGE-2	3	CDR	10.1984 - 08.2005	N/A	10° lat zones		UNI-HB/FMI
LMZ_HALOE		HALOE	3	CDR	10.1991 - 09.2005	N/A	10° lat zones		UNI-HB/FMI
LMZ_SMR (*)		SMR (*)	3	CDR (*)	07.2001 - 08.2014 (*)	N/A (*)	10° lat zones		UNI-HB/FMI
LMZ_OSIRIS		OSIRIS	3	ICDR	11.2001 - 12.2020	Annually with 3 months delay	10° lat zones		UNI-HB/FMI
LMZ_ACE		ACE	3	ICDR	02.2004 - 12.2020		10° lat zones		UNI-HB/FMI
LMZ_SABER		SABER	3	ICDR	01.2002 - 11.2020		10° lat zones		UNI-HB/FMI
LMZ_MLS		MLS	3	ICDR	08.2004 - 11.2020		10° lat zones		UNI-HB/FMI
LMZ_OMPS		OMPS-LP	3	ICDR	02.2012 - 12.2020		10° lat zones		UNI-HB/FMI
LMZ_MERGED		(2)	3	ICDR	10.1984 - 12.2020		10° lat zones		FMI
LP_MERGED		(3)	3	ICDR	11.2001 - 12.2020		10°x20°		FMI

TC Total column monthly gridded average product
NP Nadir profile monthly gridded average product

LP Limb profile monthly gridded average product
LMZ Limb monthly zonal profile average product

(*) SMR is still in operation but the L1 data processing has been interrupted. It may resume later with the reprocessing of the entire data record.

(1) Merged/assimilated product based on GOME, SCIAMACHY, OMI, GOME-2A/B, BUV-Nimbus4, TOMS-Nimbus7, TOMS-EP, SBUV-7, -9, -11, -14, -16, -17, -18, -19, OMPS and TOU.
(2) Monthly zonal mean merged product (concentration and concentration anomaly) based on MIPAS, GOMOS, SCIAMACHY, SAGE-2, OSIRIS, ACE and OMPS.
(3) Latitude-longitude gridded merged product (concentration and concentration anomaly) based on MIPAS, GOMOS, SCIAMACHY and OSIRIS.

4.2 L-3 and L-4 ozone total column derived from UV-nadir sensors

This family of C3S ozone products includes Level-3 and Level-4 monthly mean total columns retrieved from nadir satellite observations. Data are from individual sensors (Table 40), merged (Table 41) or the outcome of multi-sensor reanalysis (Table 42).

Table 40. Level 3 ozone total column monthly mean from individual UV-nadir sensors.

Originating satellite instruments	Nadir-viewing sensors GOME, SCIAMACHY, GOME-2, OMPS and OMI (cf. Sections 1.1.1 to 1.1.4)
Data class	Earth Observation Data
Data product names	• TC_GOME • TC_SCIA • TC_GOME2A • TC_OMPS • TC_GOME2B • TC_OMI
Data specification document	C3S Ozone Product User Guide and Specification *[RD-24]*
Geographic coverage	The globe
Horizontal grid	1° longitude x 1° latitude
Temporal coverage	From 1995, 2002, 2004, 2007, 2012, 2013 (depending on satellite) to 2011, 2012, today (depending on satellite)
Temporal resolution	Monthly
Main variable physical nature and unit	Monthly mean ozone total column (mol.m-2)
Data format	CF-compliant NetCDF

Table 41. Level 3 ozone total column monthly mean from UV-nadir sensors (merged)

Originating satellite instruments	Nadir-viewing sensors GOME, SCIAMACHY, GOME-2 and OMI (cf. Sections 1.1.1 to 1.1.4)
Data class	Earth Observation Data
Data product name	TC_GTO-ECV
Data specification document	C3S Ozone Product User Guide and Specification *[RD-24]*
Geographic coverage	The globe
Horizontal grid	1° longitude x 1° latitude
Temporal coverage	1995 – today
Temporal resolution	Monthly
Main variable physical nature and unit	Monthly mean ozone total column (mol.m-2)
Data format	CF-compliant NetCDF

Table 42. Level 4 ozone total column monthly mean from multi-sensor reanalysis (MSR).

Originating satellite instruments	BUV-Nimbus4, TOMS-Nimbus7, TOMS-EP, SBUV-7, -9, -11, -14, -16, -17, -18, -19, GOME, SCIAMACHY, OMI, GOME-2, FY-3A and OMPS
Data class	Earth Observation Data
Data product name	TC_MSR
Data specification document	C3S Ozone Product User Guide and Specification *[RD-24]*

Geographic coverage	The globe
Horizontal grid	1° longitude x 1° latitude
Temporal coverage	1970 – 2015
Temporal resolution	Monthly
Main variable physical nature and unit	Monthly mean ozone total column (DU)
Data format	CF-compliant NetCDF

4.3 L-3 ozone total and tropospheric column derived from IASI

The C3S ozone columns retrieved from observations by IASI include Level-3 monthly mean total and tropospheric columns (Table 43).

Table 43. Level 3 ozone total and tropospheric column monthly mean from IASI.

Originating satellite instrument	Nadir-viewing sensor IASI on board the Metop satellites (cf. Section 1.1.6)
Data class	Earth Observation Data
Data product name	• TC_IASI-A • TC_IASI-B • 06TC_IASI-A • 06TC_IASI-B
Data specification document	C3S Ozone Product User Guide and Specification *[RD-24]*
Geographic coverage	The globe
Horizontal grid	1° longitude x 1° latitude
Temporal coverage	TC_IASI-A & 06TC_IASI-A 2008-today TC_IASI-B & 06TC_IASI-B 2013-today
Temporal resolution	Monthly
Main variable physical nature and unit	• Monthly mean ozone total column (DU) • Monthly mean ozone tropospheric column (DU)
Data format	CF-compliant NetCDF

4.4 L-3 ozone profile derived from UV-nadir sensors

The C3S ozone vertical profiles derived from nadir-viewing satellites include Level-3 monthly mean data (Table 44).

Table 44. Level 3 ozone profile monthly mean from UV-nadir sensors.

Originating satellite instruments	Nadir-viewing sensors GOME, SCIAMACHY, GOME-2 and OMI (cf. Sections 1.1.1 to 1.1.4)
Data class	Earth Observation Data
Data product names	• NP_GOME • NP_SCIA • NP_GOME2A • NP_GOME2B • NP_OMI
Data specification document	C3S Ozone Product User Guide and Specification *[RD-24]*

Geographic coverage	The globe
Horizontal grid	1° longitude x 1° latitude
Vertical coverage	From surface to top of atmosphere
Vertical scale / levels	20 levels (i.e. 19 layers) in hPa, ranging from 1000 to 0.01 (adjustable)
Temporal coverage	From 1995-2017 (depending on satellite)
Temporal resolution	Monthly
Main variable physical nature and unit	• Monthly mean vertical profile of the ozone molecular number density (cm^{-3}) • Monthly mean vertical profile of the ozone volume mixing ratio (ppmv)
Data format	CF-compliant NetCDF

4.5 L-3 ozone profile derived from limb and occultation sensors

The C3S ozone vertical profiles derived from limb and occultation sensors are Level-3 monthly mean data. They include zonal averages retrieved from individual sensors (Table 45) as well as merged zonally averaged (Table 46) and gridded (Table 47) monthly mean profiles.

Table 45. Level 3 ozone profile monthly zonal mean (MZM) from limb and occultation sensors.

Originating satellite instruments	Limb and occultation sensors MIPAS, GOMOS, SCIAMACHY, SAGE-2, HALOE, OSIRIS, SMR, ACE-FTS, MLS, SABER (cf. Section 1.2)
Data class	Earth Observation Data
Data product names	• LMZ_MIPAS • LMZ_GOMOS • LMZ_SCIA • LMZ_SAGE2 • LMZ_HALOE • LMZ_OSIRIS • LMZ_SMR • LMZ_ACE • LMZ_MLS • LMZ_SABER • LMZ_OMPS
Data specification document	C3S Ozone Product User Guide and Specification *[RD-24]*
Geographic coverage	The globe
Horizontal grid	10°-width latitude zones
Vertical coverage	Instrument-specific
Vertical scale / levels	Altitude grid /pressure grid
Temporal coverage	From 1984, 1991, 2001, 2002, 2004 (depending on satellite) to 2005, 2012, today (depending on satellite)
Temporal resolution	Monthly
Main variable physical nature and unit	Monthly zonal mean (MZM) vertical profile of the ozone molar concentration ($mol.m^{-3}$)
Data format	CF-compliant NetCDF

Table 46. Level 3 ozone profile merged monthly zonal mean (MMZM) from limb and occultation sensors.

Originating satellite instruments	Limb and occultation sensors MIPAS, GOMOS, SCIAMACHY, SAGE-2, OSIRIS, ACE-FTS, OMPS (cf. Section 1.2)
Data class	Earth Observation Data
Data product name	LMZ_MERGED
Data specification document	C3S Ozone Product User Guide and Specification *[RD-24]*
Geographic coverage	The globe
Horizontal grid	10°-width latitude zones
Vertical coverage	10 -50 km
Vertical scale / levels	Altitude grid with 1 km resolution
Temporal coverage	1984 – today
Temporal resolution	Monthly
Main variable physical nature and unit	Monthly zonal mean (MZM) vertical profile of the ozone molar concentration ($mol.m^{-3}$)
Data format	CF-compliant NetCDF

Table 47. Level 3 ozone profile merged horizontally-resolved monthly mean from limb and occultation sensors.

Originating satellite instruments	Limb and occultation sensors MIPAS, GOMOS, SCIAMACHY, OSIRIS (cf. Section 1.2)
Data class	Earth Observation Data
Data product name	LP_MERGED
Data specification document	C3S Ozone Product User Guide and Specification *[RD-24]*
Geographic coverage	The globe
Horizontal grid	10° latitude x 20° longitude
Vertical coverage	10-50 km
Vertical scale / levels	Altitude grid with 1 km resolution
Temporal coverage	2002 – today
Temporal resolution	Monthly
Main variable physical nature and unit	Monthly mean vertical profile of the ozone molar concentration ($mol.m^{-3}$)
Data format	CF-compliant NetCDF

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