TROPOMI L3 Product User Manual directionally dependent surface Lambertian-equivalent reflectivity

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authors : L. G. Tilstra
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1 Introduction

1.1 Identification

This document is identified as S5P-KNMI-L3-0302-MA.

1.2 Purpose and objective

This document is the Product User Manual (PUM) of the directionally dependent Lambertian-equivalent reflectivity (DLER) of the Earth's surface derived from observations by TROPOMI. The purpose of this PUM is to present the data format used for the data record, and to explain and describe the contents of the fields contained in the database file. The document is maintained during the development phase of the data product in the context of the S5p+I project. Several updates of the document are planned.

1.3 Document overview

The structure of this PUM is as follows. In section 2 applicable, standard and reference documents are listed. Section 3 introduces terms and definitions used in this PUM, along with a list of acronyms and abbreviations that are used throughout the PUM. Section 4 provides a reference to a general description of the TROPOMI instrument. Section 5 introduces the heritage surface LER databases that are available for validation. The TROPOMI surface LER and DLER climatologies are also introduced in this section. The description of the surface DLER database is outlined in section 6. This includes a description of the parameterisation used to describe the anisotropy of the surface reflection. Product quality is discussed briefly in section 7. This PUM ends in section 8 with a short conclusion of the document.

2 Applicable and reference documents

2.1 Applicable documents

[AD1] TROPOMI Instrument and Performance Overview.
source: KNMI; **ref:** S5P-KNMI-L2-0010-RP; **issue:** 0.10.0; **date:** 2014-03-15.

2.2 Standard documents

[SD1] Space Engineering – Software.
source: ESA/ECSS; **ref:** ECSS-E-ST-40C; **issue:** 3; **date:** 2009-03-06.

2.3 Reference documents

[RD1] Terms, definitions and abbreviations for TROPOMI L01b data processor.
source: KNMI; **ref:** S5P-KNMI-L01B-0004-LI; **issue:** 3.0.0; **date:** 2013-11-08.

[RD2] Terms and symbols in the TROPOMI Algorithm Team.
source: KNMI; **ref:** S5P-KNMI-L2-0049-MA; **issue:** 2.0.0; **date:** 2016-05-17.

[RD3] R. B. A. Koelemeijer, J. F. de Haan and P. Stammes; A database of spectral surface reflectivity in the range 335–772 nm derived from 5.5 years of GOME observations. *J. Geophys. Res.*; **108** (2003) (D2); doi:10.1029/2002JD002429. URL `https://agupubs.onlinelibrary.wiley.com/doi/abs/10.1029/2002JD002429`.

[RD4] Q. L. Kleipool, M. R. Dobber, J. F. de Haan *et al.*; Earth surface reflectance climatology from 3 years of OMI data. *J. Geophys. Res.*; **113** (2008) (D18); doi:10.1029/2008JD010290. URL `https://agupubs.onlinelibrary.wiley.com/doi/abs/10.1029/2008JD010290`.

[RD5] L. G. Tilstra, O. N. E. Tuinder, P. Wang *et al.*; Surface reflectivity climatologies from UV to NIR determined from Earth observations by GOME-2 and SCIAMACHY. *J. Geophys. Res. Atmos.*; **122** (2017) (7), 4084; doi:10.1002/2016JD025940. URL `https://agupubs.onlinelibrary.wiley.com/doi/abs/10.1002/2016JD025940`.

[RD6] F. E. Nicodemus, J. C. Richmond, J. J. Hsia *et al.*; Geometrical Considerations and Nomenclature for Reflectance. *In Radiometry*; (pp. 94–145) (Jones and Bartlett Publishers, Inc., USA., 1992).

[RD7] L. G. Tilstra, O. N. E. Tuinder, P. Wang *et al.*; Directionally dependent Lambertian-equivalent reflectivity (DLER) of the Earth's surface measured by the GOME-2 satellite instruments. *Atmos. Meas. Tech.*; **14** (2021) (6), 4219; doi:10.5194/amt-14-4219-2021. URL `https://amt.copernicus.org/articles/14/4219/2021/`.

[RD8] D. F. Heath, A. J. Krueger, H. A. Roeder *et al.*; The Solar Backscatter Ultraviolet and Total Ozone Mapping Spectrometer (SBUV/TOMS) for NIMBUS G. *Opt. Eng.*; **14** (1975) (4), 323; doi:10.1117/12.7971839. URL `https://doi.org/10.1117/12.7971839`.

[RD9] J. R. Herman and E. A. Celarier; Earth surface reflectivity climatology at 340–380 nm from TOMS data. *J. Geophys. Res.*; **102** (1997) (D23), 28003; doi:10.1029/97JD02074. URL `https://agupubs.onlinelibrary.wiley.com/doi/abs/10.1029/97JD02074`.

[RD10] J. P. Burrows, M. Weber, M. Buchwitz *et al.*; The Global Ozone Monitoring Experiment (GOME): Mission concept and first scientific results. *J. Atmos. Sci.*; **56** (1999) (2), 151; doi:10.1175/1520-0469(1999)056<0151:TGOMEG>2.0.CO;2. URL `https://doi.org/10.1175/1520-0469(1999)056<0151:TGOMEG>2.0.CO;2`.

[RD11] P. F. Levelt, G. H. J. van den Oord, M. R. Dobber *et al.*; The ozone monitoring instrument. *IEEE Trans. Geosci. Remote Sens.*; **44** (2006) (5), 1093; doi:10.1109/TGRS.2006.872333. URL `https://ieeexplore.ieee.org/document/1624590`.

[RD12] R. Munro, R. Lang, D. Klaes *et al.*; The GOME-2 instrument on the Metop series of satellites: instrument design, calibration, and level 1 data processing – an overview. *Atmos. Meas. Tech.*; **9** (2016) (3), 1279; doi:10.5194/amt-9-1279-2016. URL `https://www.atmos-meas-tech.net/9/1279/2016/`.

[RD13] GOME-2 surface LER product – Algorithm Theoretical Basis Document.
source: KNMI; **ref:** SAF/AC/KNMI/ATBD/003; **issue:** 4.1; **date:** 2023-01-05.

[RD14] H. Bovensmann, J. P. Burrows, M. Buchwitz *et al.*; SCIAMACHY: Mission objectives and measurement modes. *J. Atmos. Sci.*; **56** (1999) (2), 127; doi:10.1175/1520-0469(1999)056<0127:SMOAMM>2.0.CO;2. URL `https://doi.org/10.1175/1520-0469(1999)056<0127:SMOAMM>2.0.CO;2`.

[RD15] L. G. Tilstra, M. de Graaf, I. Aben *et al.*; In-flight degradation correction of SCIAMACHY UV reflectances and Absorbing Aerosol Index. *J. Geophys. Res.*; **117** (2012) (D6); doi:10.1029/2011JD016957. URL `https://agupubs.onlinelibrary.wiley.com/doi/abs/10.1029/2011JD016957`.

[RD16] TROPOMI ATBD of the directionally dependent surface Lambertian-equivalent reflectivity.
source: KNMI; **ref:** S5P-KNMI-L3-0301-RP; **issue:** 2.0.0; **date:** 2023-08-29.

[RD17] A. Lorente, K. F. Boersma, P. Stammes *et al.*; The importance of surface reflectance anisotropy for cloud and NO_2 retrievals from GOME-2 and OMI. *Atmos. Meas. Tech.*; **11** (2018) (7), 4509; doi:10.5194/amt-11-4509-2018. URL `https://www.atmos-meas-tech.net/11/4509/2018/`.

[RD18] S5p+I – Requirements Baseline Document.
source: KNMI, GRASP, Catalysts; **ref:** D1-RBD; **issue:** 1.0; **date:** 2019-10-09.

[RD19] TROPOMI validation report of the directionally dependent surface Lambertian-equivalent reflectivity.
source: KNMI; **ref:** S5P-KNMI-L3-0401-RP; **issue:** 1.2.0; **date:** 2022-01-14.

2.4 Electronic references

[ER1] URL `https://www.temis.nl/surface/albedo/toms_ler.php`.

[ER2] URL `https://www.temis.nl/surface/albedo/gome_ler.php`.

[ER3] URL `https://www.temis.nl/surface/albedo/omi_ler.php`.

[ER4] URL `https://www.temis.nl/surface/albedo/scia_ler.php`.

[ER5] URL `https://www.temis.nl/surface/albedo/gome2_ler.php`.

3 Terms, definitions and abbreviated terms

Terms, definitions and abbreviated terms that are used in the documentation of the TROPOMI L0-1b data processor are described in [RD1]. Terms, definitions and abbreviated terms for TROPOMI Level 2 algorithms are described in [RD2]. Terms, definitions and abbreviated terms specific for this document are defined below.

3.1 Terms and definitions

There are no document specific terms and definitions.

3.2 Acronyms and abbreviations

AAI	Absorbing Aerosol Index
ATBD	Algorithm Theoretical Baseline Document
BRDF	Bidirectional Reflectance Distribution Function
BSA	Black-Sky Albedo
CAMS	Copernicus Atmosphere Monitoring Service
CF	Climate and Forecast metadata conventions
DAK	Doubling-Adding KNMI
DARIUS	Development of Advanced Retrieval of Aerosol and Surface Properties from S5P
DLER	Directionally dependent Lambertian-Equivalent Reflectivity
DU	Dobson Units, 2.69×10^{16} molecules cm^{-2}
ECMWF	European Centre for Medium-Range Weather Forecast
ENVISAT	Environmental Satellite
EOS-Aura	Earth Observing System – Aura satellite
EPS-SG	EUMETSAT Polar System – Second Generation
ERS	European Remote Sensing Satellite
ESA	European Space Agency
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
FOV	Field-of-View
FRESCO	Fast Retrieval Scheme for Clouds from the Oxygen A band
GMTED2010	Global Multi-resolution Terrain Elevation Data 2010
GOME	Global Ozone Monitoring Experiment
GRASP	Generalized Retrieval of Atmosphere and Surface Properties
HDF	Hierarchical Data Format
HITRAN2008	High-Resolution Transmission molecular absorption database, 2008 edition
IR	Infrared
ISRF	Instrument Spectral Response Function
KNMI	Koninklijk Nederlands Meteorologisch Instituut
LER	Lambertian-Equivalent Reflectivity
LUT	Look-Up Table
L2OP	Level-2 Operational Processor
L2PP	Level-2 Prototype Processor
MERIS	Medium Resolution Imaging Spectrometer
METOP	Meteorological Operational Satellite
MLS	Mid-Latitude Summer
NASA	National Aeronautics and Space Administration
NETCDF	Network Common Data Form, NetCDF
NIR	Near-Infrared

NISE	Near-real-time Ice and Snow Extent
NRT	Near-Real-Time
OMI	Ozone Monitoring Instrument
RAA	Relative Azimuth Angle
RMSE	Root-Mean-Square Error
RTM	Radiative Transfer Model
SAA	Solar Azimuth Angle
SCIAMACHY	Scanning Imaging Absorption Spectrometer for Atmospheric Chartography
Suomi NPP	Suomi National Polar-orbiting Partnership
SW	Software
SWIR	Short-Wavelength Infrared
SZA	Solar Zenith Angle
S5	Sentinel-5 mission
S5P	Sentinel-5 Precursor mission
TBA	To be Added
TBC	To be Confirmed
TBD	To be Defined
TOA	Top-of-Atmosphere
TOMS	Total Ozone Mapping Spectrometer
TROPOMI	Tropospheric Monitoring Instrument
UTC	Coordinated Universal Time
UV	Ultraviolet
UVNS	Ultraviolet Visible Near-infrared Shortwave spectrometer
VAA	Viewing Azimuth Angle
VIIRS	Visible Infrared Imaging Radiometer Suite
VIS	Visible
VZA	Viewing Zenith Angle

4 TROPOMI instrument description

A description of the TROPOMI instrument and performance can be found in [AD1].

5 Introduction to the TROPOMI DLER database

5.1 Background

Surface reflectivity databases are needed for cloud, aerosol and trace gas retrievals. Examples are the retrieval of trace gases such as ozone, NO_2, BrO, CH_2O, H_2O, CO_2, CO, and CH_4, and of cloud information and aerosol optical depth. The TROPOMI surface DLER product is the directionally dependent Lambertian-equivalent reflectivity (LER) of the Earth's surface observed by TROPOMI. It is the improved follow-up of earlier surface LER databases based on observations performed by GOME-1 (on ERS-2) [RD3], OMI (on the Aura satellite) [RD4], as well as SCIAMACHY (on Envisat) and GOME-2 (on the MetOp satellites) [RD5]. In this chapter, the term "surface reflectivity database" refers to global climatologies of surface albedo, available for several wavelength bands and for each month. The databases are generally extracted from several years of data and the term "surface reflectivity database" therefore always refers to a L4 product.

5.2 Heritage

The heritage from the traditional surface LER databases is described in section 5.2.1. These databases adhere to the principle of Lambertian surface reflection, which means that they completely disregard the fact that surface reflection is described by a bi-directional reflectance distribution function (BRDF) [RD6] which takes into account the dependence on the incoming and outgoing directions of the light reflected by the surface. Lambertian surface reflection is by definition non-directional. A directionally dependent LER (acronym: DLER) was first derived for the GOME-2 instrument [RD7]. This database will be discussed in section 5.2.2.

5.2.1 Lambertian-equivalent reflectivity (LER) databases

One of the first surface reflectivity databases retrieved using UV satellite remote sensing techniques is the Total Ozone Mapping Spectrometer (TOMS) [RD8] surface LER database [RD9]. The retrieved reflectivity is the so-called Lambertian-equivalent reflectivity (LER) of the surface found from scenes which are assumed to be cloud free. The retrieval method relies on the removal of the (modelled) atmospheric contribution from the (observed) top-of-atmosphere (TOA) reflectance. In this approach the surface is defined to behave as a Lambertian reflector. The TOMS surface LER database, which is provided in a spatial grid of $1.25^\circ \times 1.0^\circ$, was retrieved for 340 and 380 nm only, which severly limits its usefulness.

The GOME-1 [RD10] surface reflectivity database provides the surface LER on a $1.0^\circ \times 1.0^\circ$ grid for 11 wavelength bands between 335 and 772 nm [RD3]. Although this is already quite an improvement with respect to the TOMS surface LER database, the database is still limited in quality by the low number of measurements from which the surface LER had to be extracted and the large GOME footprint size (see Table 1). In particular, pixels over sea are often affected by residual cloud contamination. In these cases the surface LER was retrieved from scenes which were not sufficiently cloud free, evidenced by LER values at 772 nm exceeding 0.05 [RD3]. In other cases, e.g. snow surfaces, the surface LER was retrieved from a few measurements which were not representative for the entire month.

A large improvement on these points is the OMI surface reflectivity database [RD4]. First, the OMI instrument [RD11] has a much smaller footprint size (24 $\times$ 13 km^2 at nadir) combined with a larger global coverage (see Table 1). This leads to better statistics and results in a higher accuracy for the surface LER retrieval. Second, the higher number of measurements allows for inspecting the distribution of scene LERs for each grid cell, and for making a more sophisticated selection of representative (cloud-free) scenes instead of directly taking the minimum scene LER value like in the case of the TOMS and GOME-1 databases. Third, the provided OMI surface LER database has a higher spatial resolution of $0.5^\circ \times 0.5^\circ$. The limiting factor is the OMI wavelength range. The longest wavelength in the OMI surface LER database is 499 nm.

The GOME-2 series of satellite instruments [RD12] does not have the limitations of the above instruments and therefore can be used to create a better surface LER database. The GOME-2 instrument has the spectral range of GOME but a much smaller footprint (80 $\times$ 40 km^2) which is constant over the full swath width. The number of measurements that are available per longitude/latitude cell in the database grid is smaller than that of OMI, but enough to perform a statistical analysis on the distribution of retrieved scene LERs. The intrinsic spatial resolution of the GOME-2 surface LER database is $1.0^\circ \times 1.0^\circ$ [RD5], except near the coastlines and for certain region such as snow covered mountain ranges where it is $0.25^\circ \times 0.25^\circ$ [RD7, RD13].

The SCIAMACHY instrument [RD14] is comparable to the GOME-2 instrument, but covers a much larger spectral range. The derived SCIAMACHY surface LER database offers 34 wavelength bands between 328 and 2314 nm [RD5]. The main advantage of the GOME-2 and SCIAMACHY surface LER databases with respect

Surface LER database →	**TOMS**	**GOME-1**	**OMI**	**SCIAMACHY**	**GOME-2**	**Sentinel-5P**
surface reflectivity type	LER	LER	LER	LER	LER / DLER	LER / DLER
dataset time range [1]	1978–1993	1995–2000	2004–2007	2002–2012	2007→	2018→
selected wavelength bands	2	11	23	34	27	21
wavelength range covered [nm]	340–380	335–772	328–499	328–2314	328–772	328–2314
band width [nm]	1.0	1.0	1.0	1.0	1.0	1.0
spatial resolution [°lon × °lat]	1.25 × 1.0	1.0 × 1.0	0.5 × 0.5	0.5 × 0.5 [2]	0.25 × 0.25 [2]	0.125 × 0.125
reference	[RD9]	[RD3]	[RD4]	[RD5]	[RD5, RD7]	[RD16]
instrument	TOMS	GOME	OMI	SCIAMACHY	GOME-2	TROPOMI
satellite	Nimbus-7	ERS-2	Aura	Envisat	MetOp-A/B/C	Sentinel-5P
equator crossing time (LT)	12:00	10:30	13:45	10:00	09:30	13:30
dayside flight direction	S→N	N→S	S→N	N→S	N→S	S→N
number of days for global coverage	1	3	1	6	1.5	1
pixel size at nadir [km × km]	50 × 50	320 × 40	24 × 13	60 × 30	80 × 40	5.6 × 3.6 [3]
number of usable pixels per orbit	∼12000	∼1300	∼83000	∼4000	∼11000	∼1300000

Table 1: Characteristics and properties of the surface LER databases, and of the satellite instruments from which they are derived. Wavelength band information can be found in Table 2.

to the OMI surface LER database is the wider wavelength range of the GOME-2 and SCIAMACHY instrument. Additionally, the retrieval algorithm uses aerosol information, available via the Absorbing Aerosol Index (AAI) product [RD15], to filter out scenes with large amounts of aerosols, as these scenes can result in inaccurate values of the retrieved surface LER. This filtering is especially important for locations over desert areas.

The SCIAMACHY and GOME-2 surface LER databases are derived by similar retrieval codes using similar techniques. Together with the OMI surface LER database they provide all the heritage available to develop the TROPOMI surface DLER database. Table 1 summarises the properties of the surface reflectivity databases discussed in this section. References to papers and other sources of information are also provided. Table 2 provides detailed information on the wavelength bands that are contained in the surface LER databases.

5.2.2 Directional LER databases

The concept of a directional LER was first introduced to the GOME-2 surface DLER database [RD7]. The GOME-2 surface DLER database provides, next to the traditional LER database, a DLER database which is essentially a function of the viewing direction (and of month, wavelength, latitude, and longitude). For the GOME-2 surface DLER database, the difference between DLER and LER is the largest for the west viewing geometries. For example, at 772 nm the surface DLER for a vegetated scene over Amazonia can be twice as large in the west viewing direction as in the east viewing direction [RD17]. The traditional LER databases discussed in section 5.2.1 completely miss this directional dependence, and generally present a value which is very close to the minimum of the DLER over all viewing angles.

5.2.3 Links to the heritage LER databases

The heritage LER databases can be download from the following locations:

- TOMS surface LER : [ER1]
- GOME-1 surface LER : [ER2]
- OMI surface LER : [ER3]
- SCIAMACHY surface LER : [ER4]
- GOME-2 surface DLER : [ER5]

[1] The longer the time period, the larger the number of times a certain region has been observed. This increases the chances of having observed this region under clear-sky conditions. [2] The *intrinsic* resolution is in most cases 1.0°×1.0°. [3] The TROPOMI spatial sampling in the along track direction was changed from 7.2 km to the indicated 5.6 km on 6 August 2019, at the start of orbit 9388.

5.3 TROPOMI DLER database

The TROPOMI surface DLER database is in many aspects a huge step forward compared to the other databases described in Table 1. The spatial resolution of the TROPOMI DLER database will be $0.125° \times 0.125°$. This high spatial resolution is made possible by the small TROPOMI footprint size of 5.6 $\times$ 3.6 km^2. The smaller footprint size also results in a much larger number of cloud-free pixels that may be collected over the course of a given time period. This is beneficial for the stability and the quality of the retrieved DLER spectra. Figure 1 provides a good indication of the spatial resolution for the surface LER climatologies derived from GOME-1, GOME-2, and TROPOMI. Obviously, the higher spatial resolution of TROPOMI is an important improvement.

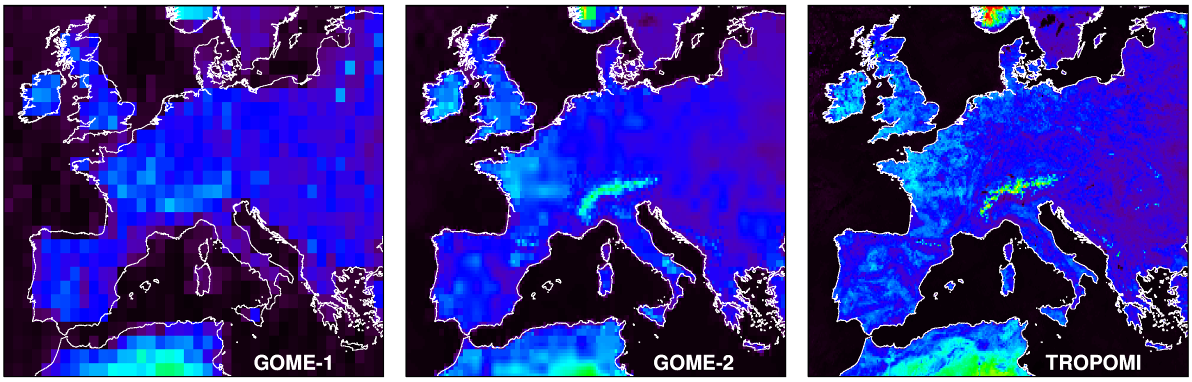

Figure 1: Surface LER in March over Europe according to the GOME-1, GOME-2, and TROPOMI databases.

Another step forward is the way in which the cloud screening is performed. For all surface LER databases listed in Table 1 the cloud screening is based on statistical methods. The advantage of this is that external cloud information is not required. The disadvantage is the risk of residual cloud contamination for areas known to be nearly always covered by persistent cloud decks. Another disadvantage is the high computational effort needed: all scenes need to be handled at once, cloud-free or not, which can be quite a task when handling a satellite instrument like TROPOMI with more than a million footprints per orbit (see Table 1).

For TROPOMI the cloud screening will be based primarily on the S5P NPP-VIIRS cloud product. The NPP-VIIRS product is based on observations performed by the VIIRS instrument onboard the Suomi NPP satellite. The S5P and NPP satellites are kept in a “loose” formation in very similar orbits, resulting in only a relatively small time difference (currently the difference is approximately 3 minutes, reduced from 5 minutes at the start of the mission). The VIIRS cloud information is provided for each individual TROPOMI footprint. More precisely, the product provides cloud information for four sets of boxes surrounding the TROPOMI measurement footprint. For our purpose, we use the nominal size of these boxes, corresponding to the smallest FOV, which matches precisely the size of the TROPOMI footprints as found in the L1 and L2 products. Separate S5P NPP-VIIRS products are provided for spectral band 3, 6, and 7. This means that there is collocated cloud information available for all used TROPOMI spectral bands (these are: bands 3/4, 5/6, and 7).

Another major improvement is in the fact that for determining the TROPOMI surface DLER, the information can be studied as a function of viewing angle without the use of viewing-angle containers. For the GOME-2 DLER, these viewing-angle containers are needed to be able to perform the statistical cloud screening [RD7]. The fact that the “container” approach is not needed for deriving the TROPOMI surface DLER is, therefore, a direct result of the decision to use the S5P NPP-VIIRS cloud product for the cloud screening.

Generally speaking, the approach that was used for the GOME-2 and SCIAMACHY surface reflectivity databases was followed closely and applied in the TROPOMI surface DLER retrieval algorithm.

5.4 Wavelength bands

In Table 2 we list the wavelength bands of the surface reflectivity databases discussed in section 5.2, and their application. As can be seen, the selection of the wavelength bands for TROPOMI was influenced largely by the already existing surface LER databases. Below 325 nm the surface contribution to the TOA reflectance is low, which prevents an accurate retrieval of the surface LER below this wavelength. The TROPOMI surface LER wavelength band at 328 nm is retrieved, but for the time being only for testing and monitoring purposes. It will not be part of the TROPOMI surface DLER database unless it is proven to be of sufficient quality. Sufficient quality means that the requirements set in the Requirements Baseline Document [RD18] need to be met.

Band	TOMS	GOME	OMI	SCIAMACHY	GOME-2	TROPOMI	Application
328			+ (1)	+ (1)	+ (1)	+ (1)	ozone, HCHO, SO_2
335		+	+	+	+	+	ozone, HCHO
340	+			+	+	+	cloud, aerosol, HCHO, BrO
342			+				cloud, aerosol, HCHO, BrO
345			+				cloud, aerosol, HCHO, BrO
354			+	+	+	+	cloud, aerosol, HCHO, BrO, OClO
367			+	+	+	+	cloud, aerosol, OClO
372			+				cloud, aerosol, OClO
376			+				cloud, aerosol, OClO
380	+	+	+	+	+	+	cloud, aerosol, OClO
388			+	+	+	+	cloud, aerosol, OClO
402						+	cloud, aerosol
406			+				cloud, aerosol
416		+	+		+	+	cloud, aerosol
418			+				cloud, aerosol
425			+	+	+	+	cloud, aerosol, NO_2
440		+	+	+	+	+	cloud, aerosol, NO_2
442			+				cloud, aerosol, NO_2
452			+				cloud, aerosol, NO_2
463		+	+	+	+	+	cloud, aerosol, NO_2, O_2-O_2
471			+				cloud, aerosol, NO_2, O_2-O_2
477			+ (2)				cloud, aerosol, NO_2, O_2-O_2
488			+				cloud, aerosol, NO_2, O_2-O_2
494		+	+	+	+	+	cloud, aerosol, NO_2, O_2-O_2
499			+				cloud, aerosol
510				+	+		cloud, aerosol
526				+	+		cloud, aerosol
546				+	+		cloud, aerosol
555		+		+	+		cloud, aerosol
564				+	+		cloud, aerosol, O_2-O_2
585					+		cloud, aerosol, O_2-O_2, H_2O
610		+			+		cloud, aerosol, H_2O
614				+			cloud, aerosol, H_2O
640				+	+		cloud, aerosol, H_2O
670		+		+	+	+	cloud, aerosol, H_2O, O_2-B
685				+	+	+	cloud, aerosol, H_2O, O_2-B
697				+	+	+ (3)	cloud, aerosol, H_2O, O_2-B
712				+	+	+ (3)	cloud, aerosol, H_2O, O_2-B
747					+	+	cloud, aerosol, H_2O
758		+		+	+	+	cloud, aerosol, O_2-A
772		+		+	+	+	cloud, aerosol, O_2-A
862				+			cloud, aerosol, H_2O
875				+			cloud, aerosol, H_2O

1030				+			cloud, aerosol, H_2O
1053				+			cloud, aerosol, H_2O
1245				+			cloud, aerosol, H_2O
1557				+			cloud, aerosol, H_2O, CH_4, CO_2
1593				+			cloud, aerosol, H_2O, CH_4, CO_2
1630				+			cloud, aerosol, H_2O, CH_4, CO_2
1670				+			cloud, aerosol, H_2O, CH_4, CO_2
2314				+		+ (4)	cloud, aerosol, H_2O, CH_4, CO

Table 2: Wavelength bands of the surface LER databases discussed in this paper, and their atmospheric applications. All wavelength bands are located outside strong gaseous absorption bands in order to avoid complicated modeling of the radiative transfer involved. The wavelength bands are 1 nm wide in most cases.

For most of the wavelength bands the exact central wavelength is not very critical, and the exact central position in the algorithm setup is exactly that as shown in Table 2. Exceptions are the 697 and 712-nm TROPOMI DLER wavelength bands. These have been given a central wavelength of 696.97 and 712.70 nm, respectively. The positions of these wavelength bands are based on very precise spectral calculations with the goal to minimise the impact of surrounding water vapour absorption bands. The width of the wavelength bands will be one nm in most cases. Exceptions are the wavelength bands at 697, 712, and 2314 nm. The 697 and 712-nm wavelength bands will have a bandwidth of 0.3 nm. The 2314-nm wavelength band will have a bandwidth of 0.5 nm. The bandwidths that are defined for TROPOMI are in line with those used in the earlier databases.

(1) Retrieval of the surface LER below 330 nm is challenging because of the small contribution of the surface to the TOA reflectance. (2) The wavelength band at 477 nm is ill-positioned because here the retrieved (OMI) surface LER is affected by O_2-O_2 absorption. (3) The 697 and 712-nm wavelength bands are surrounded by water vapour absorption bands. Their bandwidth is 0.3 nm and their exact positions are 696.97 and 712.70 nm, respectively. (4) The 2314-nm wavelength band will have a bandwidth of 0.5 nm.

6 Product description

6.1 Product file

The TROPOMI surface DLER database is contained in a file typically named as:

`TROPOMI_Sentinel-5P_0125x0125_surface_DLER_v2.0.nc` (15 Gb)

The file format of the TROPOMI surface DLER product file is NetCDF-4. The fields that are contained in the product files are presented in Figure 2 and are discussed in sections 6.2 and 6.3.

Name	Long Name	Type
TROPOMI_Sentinel-5P_0125x0125_surface_DLER_v2.0.nc	Surface Lambertian-equivalent reflectivity (LER) observed by TROPOMI	Local File
age_clear	age of the observations in units of months	Geo2D
age_snice	age of the observations in units of months	Geo2D
flag	flag indicating the processing history	Geo2D
latitude	latitude of the centre of the grid cell	1D
longitude	longitude of the centre of the grid cell	1D
minimum_LER_clear	surface LER retrieved for snow/ice-free conditions	Geo2D
minimum_LER_snice	surface LER retrieved for snow/ice conditions	Geo2D
month	name of the month	—
polynomial_coefficients_clear	polynomial coefficients for the directionally dependent surface LER for snow/ice-free surfaces	Geo2D
polynomial_coefficients_index	index of the polynomial coefficients	1D
polynomial_coefficients_snice	polynomial coefficients for the directionally dependent surface LER for snow/ice surfaces	Geo2D
uncertainty_clear	estimated uncertainty for snow/ice-free conditions	Geo2D
uncertainty_snice	estimated uncertainty for snow/ice conditions	Geo2D
wavelength	central wavelength of the wavelength band	1D

Figure 2: Contents of the TROPOMI surface DLER NetCDF file.

6.2 Contents of the product file

The product_version of the TROPOMI surface DLER database described in this document is version 2.0. The product_format_version for this version of the DLER database is 0.4. The contents of the DLER database file – variable names, units, dimensions, and descriptions – is listed in Table 3. Each variable has a series of attributes providing complementary information to the user. Possible attributes are listed in Table 4.

The “wavelength” field is an array listing the central wavelengths of each of the wavelength bands in nanometers. The width of the wavelength bands is typically 1.0 nm [RD16]. The number of wavelength bands (nwav) is 21. The “longitude” and “latitude” arrays contain the centre longitudes or latitudes of the various grids contained in the product. The dimensions of the grids in the database file are in most cases defined by nlon=2880, nlat=1440, nwav=21, nmon=12.

The “minimum_LER_clear” and “minimum_LER_snice” fields hold the surface LER grids retrieved using the MIN-LER approach. The dimensions of the matrices are nmon $\times$ nwav $\times$ nlon $\times$ nlat. As explained in the ATBD [RD16], the MIN-LER approach determines the surface LER in the traditional way in which the minimum scene LER of cloud-free scenes that is found over time for a certain location is assumed to be representative for the surface LER. The “minimum_LER_clear” is retrieved with the intent to record the surface LER for scenes that are not containing snow or ice surfaces. Likewise, the “minimum_LER_snice” field is determined specifically to represent snow/ice-containing scenes, when possible. It is up to the user to decide which of the two fields is representative for the situation at hand. This requires external snow/ice information.

An integer, bitwise quality flag is provided in the “flag” field. The dimension of the matrix is nmon $\times$ nwav $\times$ nlon $\times$ nlat. Table 5 explains the meaning of the flag values and provides the flag masks. Note that some of the flag values relate to the “clear” field and some to the “snice” field, as indicated by the third column of Table 5. The ATBD [RD16] provides a more complete description of the quality flag.

The fields “age_clear” and “age_snice” indicate the age (in units of months) of the values provided in the grids. The dimensions of the matrices are nmon $\times$ nwav $\times$ nlon $\times$ nlat. An age of zero is optimal, since it indicates that the retrieval was able to produce a value based on the observations of the month at hand. If the age is negative or positive, then it indicates that the retrieval was not successful. The age then indicates the month which provided a donor value. The age can be any number between –6 and +6 months.

The fields “uncertainty_clear” and “uncertainty_snice” provide an indication of the uncertainty in the retrieved surface LER values. They are derived using equation (22) of the ATBD [RD16]. The dimensions of the matrices are nmon $\times$ nwav $\times$ nlon $\times$ nlat.

The other fields “polynomial_coefficients_index”, “polynomial_coefficients_minimum_LER_clear”, and “polynomial_coefficients_minimum_LER_snice” mentioned in Table 3 are explained in the next section.

Name	Unit	Dimensions	Description / long name
month	–	12	name of the month
wavelength	nm	21	central wavelength of the wavelength band
latitude	degrees	1440	latitude of the centre of the grid cell
longitude	degrees	2880	longitude of the centre of the grid cell
age_clear	months	12 x 21 x 2880 x 1440	age of the observations in units of months
age_snice	months	12 x 21 x 2880 x 1440	age of the observations in units of months
flag	–	12 x 21 x 2880 x 1440	flag indicating the procesing history
minimum_LER_clear	–	12 x 21 x 2880 x 1440	surface LER retrieved for snow/ice-free conditions
minimum_LER_snice	–	12 x 21 x 2880 x 1440	surface LER retrieved for snow/ice conditions
uncertainty_clear	–	12 x 21 x 2880 x 1440	estimated uncertainty for snow/ice-free conditions
uncertainty_snice	–	12 x 21 x 2880 x 1440	estimated uncertainty for snow/ice conditions
polynomial_coefficients_index	–	4	index of the polynomial coefficients
polynomial_coefficients_clear	–	12 x 21 x 2880 x 1440 x 4	polynomial coefficients for the directionally dependent surface LER for snow/ice-free surfaces
polynomial_coefficients_snice	–	12 x 21 x 2880 x 1440 x 4	polynomial coefficients for the directionally dependent surface LER for snow/ice surfaces

Table 3: List of variables stored in the TROPOMI surface DLER file.

Attribute	Description
comment	miscellaneous information about the data or methods used to produce it
coordinates	identifies auxiliary coordinate variables, providing a connection between data and geolocation
standard_name	a standard name that references a description of a variable in the standard name table
long_name	a longer name describing the variable more clearly
flag_values	a list of the flag values; to be used in combination with flag_masks and flag_meanings
flag_meanings	use in combination with flag_values to find the meaning of each flag value
flag_masks	a list of the flag masks; to be used to find the flag values raised in the flag
_FillValue	value to represent missing or undefined data
units	unit of the variable

Table 4: List of possible attributes associated to the variables shown in Table 3.

flag value	flag mask	field	meaning of flag
1	7	CLEAR	data are ok; no corrections applied
2	7	CLEAR	residual cloud contamination above ocean detected – replaced by nearby cloud-free cell
3	7	CLEAR	residual cloud contamination above ocean detected – no suitable replacement could be found (the pixel remains cloud contaminated and/or receives the LER spectrum of a less than optimal donor cell)
4	7	CLEAR	missing data for polar regions which are observed only part of the year – filled in using nearest month with reliable surface LER data
5	7	CLEAR	missing data throughout the entire year
6	7	CLEAR	suspect surface LER value retrieved
8	8	CLEAR	empty cell was replaced by grid cell from SNICE field
16	112	SNICE	data are ok; no corrections applied
32	112	SNICE	residual cloud contamination above ocean detected – replaced by nearby cloud-free cell
48	112	SNICE	residual cloud contamination above ocean detected – no suitable replacement could be found (the pixel remains cloud contaminated and/or receives the LER spectrum of a less than optimal donor cell)
64	112	SNICE	missing data for polar regions which are observed only part of the year – filled in using nearest month with reliable surface LER data
80	112	SNICE	missing data throughout the entire year
96	112	SNICE	suspect surface LER value retrieved
128	128	SNICE	empty cell was replaced by grid cell from CLEAR field

Table 5: Definition of the quality flag that is provided along with the TROPOMI surface DLER database.

6.3 Directionally dependent surface LER (DLER)

The surface DLER is parameterised as a function of the viewing angle (denoted as θ_v) in the following way:

$$A_\mathrm{DLER} = A_\mathrm{LER} + c_0 + c_1 \cdot \theta_\mathrm{v} + c_2 \cdot \theta_\mathrm{v}^2 + c_3 \cdot \theta_\mathrm{v}^3 \ , \tag{1}$$

where θ_v is negative on the east side of the orbit swath ($\theta_\mathrm{v} = -\theta$), and positive on the west side of the orbit swath ($\theta_\mathrm{v} = \theta$). To be absolutely specific and to avoid potential mistakes, this is additionally shown graphically in Figure 3. The parameter A_LER refers to the "minimum_LER" fields mentioned in Table 3, and the c_0, c_1, c_2, and c_3 are the four polynomial coefficients stored in the "polynomial_coefficients_minimum_LER" fields mentioned in Table 3. The dimensions of the matrices are nmon × nwav × nlon × nlat × 4.

For water bodies the coefficients c_0, c_1, c_2, and c_3 are set to zero. They are also set to zero for coastal areas and for areas for which the surface DLER could not be retrieved. A failure to retrieve the DLER occurs when not the entire viewing angle range is covered. This happens systematically near the polar regions, for very high solar zenith angles, when part of the TROPOMI scanline has $\theta_0 < 85^\circ$ and the other part has $\theta_0 > 85^\circ$. It can also happen when a region or location is suffering from structural (persistent) cloud presence.

Since the TROPOMI surface DLER database is derived exclusively from observations taken from the ascending orbit parts of the TROPOMI orbits (see the ATBD [RD16]), the DLER expansion is only valid for the ascending orbit part of the TROPOMI (or OMI) orbit. For the descending orbit part, the DLER expansion is therefore not to be used and the user should use the standard non-directional LER field instead.

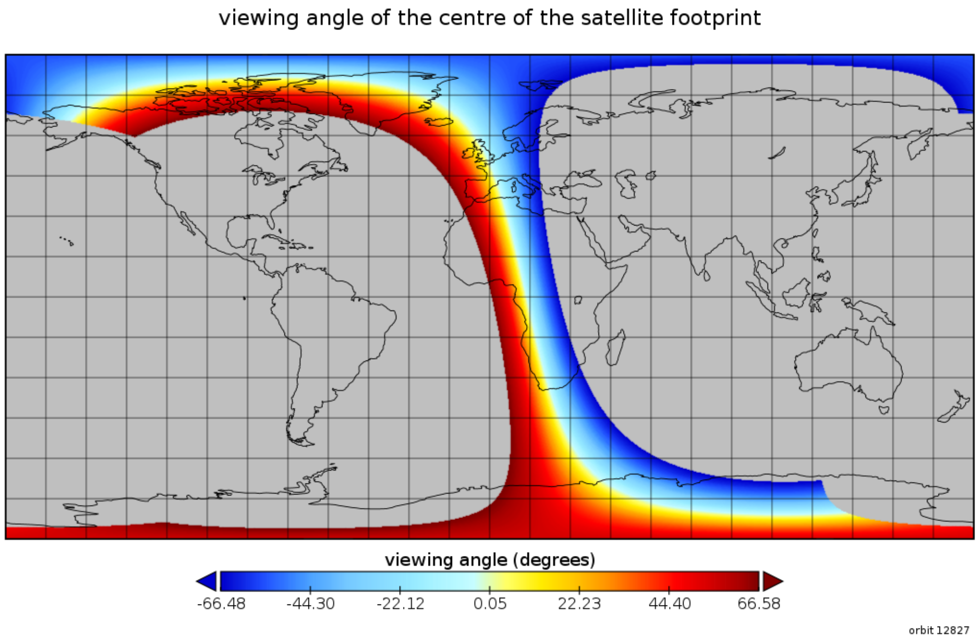

Figure 3: Definition of the viewing angle θ_v. The viewing angle θ_v is negative on the east side of the orbit swath ($\theta_v = -\theta$), and positive on the west side of the orbit swath ($\theta_v = \theta$).

7 Product quality

Please refer to the Validation Report [RD19] for information on the product quality.

8 Conclusion

This document is the Product User Manual (PUM) of the directionally dependent Lambertian-equivalent reflectivity (DLER) of the Earth's surface derived from observations by TROPOMI. The purpose of this PUM is to present the data format used for the data record, and to explain and describe the contents of the fields contained in the database file.