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S5P/TROPOMI Static input for Level 2 processors





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1 Introduction

1.1 Identification

This document, identified as S5P-KNMI-L2CO-0004-SD, describes the static input data that is required by all level 2 products for S5P/TROPOMI.

1.2 Purpose and objective

This document describes the static input data that is required by the S5P/TROPOMI level 2 processors. This includes sources for reference spectra, elevation data and surface albedo climatologies.

This document aims to harmonize assumptions and reference spectra used for the operational TROPOMI level 2 retrieval algorithms. All level 2 ATBDs are expected to include this document as an applicable document.

1.3 Document overview

In section 4 we give an overview of the spectroscopic reference data. Sections 5 and 6 describe the surface elevation data and the surface albedo reference. Sources for static a priori data are given in section 7. Finally, instrument parameters are listed in section 8.

2 Applicable and reference documents

2.1 Applicable documents

There are no applicable documents

2.2 Standard documents

There are no standard documents

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.
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3 Terms, definitions and abbreviated terms

Terms, definitions and abbreviated terms that are used in the development program for the TROPOMI L0-1B data processor are described in [RD1]. Terms, definitions and abbreviated terms for the L2 algorithms are described in [RD2]. Terms, definitions and abbreviated terms that are specific for this document can be found below.

3.1 Acronyms and Abbreviations

- CTM Chemistry Transport Model
- DEM Digital elevation map

4 Spectroscopic reference data

A large number of reference spectra can be found at the Max Planck institute in Mainz [RD3] and in the HITRAN database [RD4]. Specific references are listed below.

O₃ **reference spectrum** O₃ cross section spectrum. Possible sources include Brion *et al.* [RD5, RD6, RD7, RD8], Serdyuchenko *et al.* [RD9, RD10] and Bogumil *et al.* [RD11]. Useful references can be found through [ER1], including links to the articles by Sedyuchenko *et al* and the raw reference data.

The current baseline is Brion et al. [RD5, RD6, RD7, RD8].

Algorithms NO₂, O₃ profiles, O₃ column, SO₂ column, HCHO column.

NO₂ reference spectrum NO₂ cross section spectrum. The reference spectrum used for OMI is by Vandaele *et al.* [RD12].

Algorithms NO₂ column, SO₂ column, HCHO column.

SO₂ reference spectrum The SO₂ reference spectrum is a composite based on Bogumil *et al.* [RD11] and Hermans *et al.* [RD13]. The Bogumil data set at 203 K is used in the 310 nm to 335 nm range. For large volcanic SO₂ plumes, we switch to a spectral range between 360 nm and 390 nm. The measured SO₂ absorption bands between 360 nm and 390 nm are very noisy in the Bogumil *et al.* data. Therefore the original Bogumil *et al.* cross-sections are replaced by the cross-sections measured by Hermans *et al.* As the Hermans data set is not provided at 203 K the cross-sections are extrapolated to 203 K using the temperature dependence that can be seen in the Bogumil *et al.* spectra.

Algorithms SO₂ column, HCHO column, possibly O₃ profile.

HCHO reference spectrum The baseline reference spectrum is Meller and Moortgat [RD14]. An alternative and equivalent dataset is by Chance and Orphal [RD15].

Algorithms HCHO columns.

- **BrO reference spectrum** The current baseline is to use Fleischmann *et al.* [RD16] with a reference temperature of 223 K. The following datasets might be tested:
 - Wilmouth et al. [RD17] with a reference temperature of 228 K.
 - Sander et al. [RD18] with a reference temperature of 228 K.

Algorithms SO₂ column, HCHO column.

O₂ reference spectrum O₂ cross section data, for the O₂ A- and B-band (760 nm and 688 nm). The canonical source is HITRAN [RD4], with additions from [RD19, RD20, RD21, RD22] for line-mixing and collision induced absorption. An alternative source is used in the GOSAT community based on reference measurements performed at JPL, but sadly this data is unpublished so far. We have contacted Tran *et al.* to obtain a copy of their code.

Algorithms Clouds (both the KNMI cloud support product as well as the official cloud product), aerosol layer height, CH₄

O₂–O₂ reference spectrum A new spectrum has recently been published [RD23]. This publication uses atmospheric pressures, and covers the UV wavelengths that were previously only covered by Greenblatt [RD24]. This new publication compares well with Hermans *et al.* [RD25] in the region where they overlap. When O₂–O₂ is fitted, we recommend to investigate this new publication as a data source. As a backup the combination of [RD25] and [RD24] can be used.

Algorithms SO₂ column, HCHO column.

H₂O reference spectrum H₂O vapor absorption cross section data for use in the SWIR, NIR and UV/VIS channels. The canonical source is the HITRAN [RD4]. The NIR (aerosol layer height) channel uses HITRAN as is. For the UV/VIS channels (NO₂) a reference spectrum suitable for DOAS retrieval can be generated based on HITRAN, as the water vapor absorption is sufficiently weak in this spectral region. See section 4.1 for details.

For the SWIR channel (CH₄ and CO) a different source is supplied by SRON [RD26].

Algorithms CH₄, CO, NO₂, aerosol layer height.

Liquid H₂O The retrievals NO₂ and glyoxal (OCHCHO) are affected by absorption in liquid water (H₂O_{liq}). A reference spectrum of H₂O_{liq} can be found in [RD27].

Algorithms NO₂, others TBD.

- **CH₄ reference spectrum** CH₄ cross section data. The canonical source is HITRAN [RD4] **Algorithms** CH₄, CO
- **CO reference spectrum** CO cross section data. The canonical source is HITRAN [RD4]

Algorithms CH₄, CO

Several other spectroscopic parameters will have to be defined.

- **O**₂ concentration Needed to use O₂ as a ruler for cloud and aerosol altitude. We propose to use 0.20946 based on Goody [RD28, table 1.2].
- **Solar reference spectrum** Currently described in [RD29], which combines [RD30] for 200 600 nm with a spectrum by Chance (private communication, Johan de Haan) for the range 600 1000 nm and some other sources for longer wavelengths.

There is an updated spectrum by Chance and Kurucz [RD31], the ESA document will have to be updated in due time. Toon *et al.* [RD32] have a high resolution transmission spectrum of the solar atmosphere based on observations from high altitude balloons. An initial comparison shows that the spectrum by Chance and Kurucz may still have some contamination by atmospheric absorption lines in the O₂ A-band. The effect on the retrieval of aerosol layer height is very limited.

We prefer to continue using [RD29] with the section 600-1000 nm updated using Chance and Kurucz [RD31]. The update is needed to obtain a reference spectrum where all sections can be easily referenced in peer-reviewed journals. The difference between the revisions in the solar spectra themselves is minor.

A clearer description of the high resolution solar irradiance for the SWIR channel is still needed.

- **Rayleigh optical depth** The refractive index and depolarization factors for N₂, O₂ and Ar by Bodhaine *et al.* [RD33] are used.
- **Molecular scattering phase matrix** The Rayleigh, Cabannes and rotational Raman scattering phase matrices from Stam *et al.* [RD34] are used.
- **Ring effect** Here we need to combine several sources: the high-resolution solar reference spectrum, a Stokes spectrum, and the instrument slit function. See section 4.2.

Algorithms All algorithms that use bands 1-4 (270 - 500 nm).

4.1 Note on water vapor spectrum for DOAS (NO₂)

The water vapor absorption spectrum is a line spectrum, and can not be used with DOAS. We can get away with the DOAS approximation for NO₂ because it is a very weak absorber in the visual spectral range. The spectrum is based on HITRAN [RD4], but requires a few steps to translate into a usable spectrum for DOAS.

- Use HITRAN [RD4] to simulate a reflectance spectrum for a representative H₂O vapor profile. The reflectance spectrum must be convolved with the instrument slit function.
- Use $R = R_0(1 N_s \sigma_{H_2O}(\lambda))$ with R_0 the spectrum without water vapor in the atmosphere, and N_s the slant column. By simulating both R and R_0 we can obtain $N_s \sigma_{H_2O}(\lambda)$.
- Fit a polynomial to the N_sσ_{H₂O}(λ) spectrum and subtract it to obtain a differential spectrum. Note that this spectrum is still scaled with N_s.
- Use simulations to calculate N_s, for instance

$$N_{\rm S} = \int_z m(z) n(z) \, \mathrm{d} z$$

with n(z) the number density of H₂O, and m(z) the altitude dependent airmass factor.

• Using the value for the slant column, a differential cross section for water vapor can be obtained from the scaled spectrum.

4.2 Note on Raman scattering and Ring effect

Here we need to combine several sources: the high-resolution solar reference spectrum, a Stokes- and anti-Stokes spectrum for an average atmospheric temperature (solar spectrum convolved with N_2 and O_2 rotational Raman scattering cross-sections), and the instrument slit function.

For the O_3 profile, O_3 total column, HCHO column, and SO_2 retrieval algorithms Ring spectra will be calculated internally. The O_3 profile retrieval will use the rotational Raman parameters provided by Chance and Spurr [RD35] and separate calculations using Rayleigh scattering and Cabannes scattering for the molecules in the atmosphere. The other algorithms will test and the following methods:

- Vountas et al. [RD36], using 2 Ring spectra.
- Chance and Spurr [RD35], using one Ring spectrum.
- Wagner et al. [RD37], using one Ring spectrum.

For the O_3 total column retrievals, an O_3 cross section spectrum that is smoothed or scrambled by rotational Raman scattering is also required. This will be computed internally.

4.3 Non-linear ozone absorption

The method of Pukīte *et al.* [RD38] will be used. In this method, the wavelength dependence of the O_3 slant columns in the retrieval interval is expressed as a Taylor expansion of the wavelength and the optical depth. In practice, the method adds two pseudo-cross sections to the DOAS fitting vector. For the HCHO and SO₂ retrieval algorithm, these additional spectra will be calculated internally.

5 Surface elevation

The widely used GTOPO30 elevation database is known to be inaccurate in certain areas, and a better reference is needed. For the CH₄ and CO access to ASTER [ER2] or the SRTM dataset [ER3] is requested. Unfortunately both ASTER and SRTM do not provide full global coverage, although the regions relevant for CH₄ and CO are covered. An alternative is the DEM delivered with the SDP toolkit by NASA [ER4]. The latter DEM is available at a spatial sampling of 90 and 15 arcseconds (1/40th or 1/240th of a degree, or better than 3 or 0.5 km). The dataset is complete for the 90 arcsecond spatial resolution, while Greenland and Antarctica are missing from the 15 arcsecond dataset. A final dataset is provided by the USGS in the GMTED2010 DEM [ER5]. This is a composite dataset, based mainly on the SRTM mission, but filling in data gaps with other sources.

The level 1B team would like to limit its external dependencies. This includes the surface altitude, as different level 2 developers may have different ideas for their needs. If the level 2 working group can come up with the single high quality database they would like to be used, then this may be reconsidered. As an alternative we can perform this regridding in a separate intermediate level 2 product to provide a consistent altitude reference for all level 2 products.

The DEM that is provided by the SDP toolkit [ER4] includes a surface classification (land, several types of water). This classification is also needed for a sun-glint flag. This information is *not* provided in the GMTED2010 dataset.

The current baseline for the elevation is the GMTED2010 dataset [ER5]. The baseline for the surface classification is the SDP toolkit [ER4].

6 Surface albedo

At the moment there is no surface albedo database that will cover the complete spectral range of TROPOMI. There is the GOME-1 Lambertian equivalent reflector (LER) surface albedo database [RD39], but the spatial resolution of GOME-1 is such that this database is likely cloud-contaminated.

For the wavelength range below 500 nm the OMI LER database [RD40] is probably most appropriate. A surface albedo database based on MERIS may provide the needed additional coverage for the NIR spectral range (Band 5 and 6) [RD41], even though MERIS provides a black sky albedo (BSA). The difference between a LER and BSA surface albedo can probably be neglected in the NIR spectral range.

For the SWIR channel albedo maps from SCIAMACHY can be used as a priori surface albedo.

We recommend to collect data from TROPOMI to build a new surface albedo database. Collecting this data once the instrument features are well understood (i.e. after the first level 1B reprocessing), will help to provide an alternative surface albedo database after an estimated 2 years in operation, perhaps with yearly updates thereafter.

As a baseline we propose the OMI LER database [RD40] for wavelengths smaller than 500 nm. For the NIR channel we propose to use the MERIS dataset over land, with additional coverage over sea from GOME-1 as provided by Popp *et al.* [RD41]. For the SWIR channel a priori albedo maps will be provided by SCIAMACHY.

6.1 The ADAM project

The ADAM ("A surface reflectance Database for ESA's Earth observation missions") study is expected to provide a global surface reflectance database covering 300 to 4000 nm, with 1 nm sampling, a $10 \times 10 \, \mathrm{km}^2$ spatial resolution and including variability on a $1 \times 1 \, \mathrm{km}^2$ scale. The data set is not yet publicly available. In principle this data set is interesting, but the usability of this dataset strongly depends on the quality of the atmospheric correction algorithm and the source observations used to build the database in the first place.

Early information we have seen on the production of the dataset is the following:

Source observations MODIS/Terra (morning orbit) and MODIS/Aqua (afternoon orbit). **Spectral coverage** 7 bands in the 300 nm to 4000 nm range. Which bands are used is not clear, as there are

22 bands on MODIS in this spectral range.

Spectral resolution The width of these bands ranges from 10 to 50 nm.

Limitations The shortest wavelength band on MODIS covers 405-420 nm.

This raises serious questions on the usability of the dataset for atmospheric retrievals:

- 1. How is the wavelength range below 400 nm covered? Is this done by extrapolation?
- 2. How can a spectral sampling of 1 nm be obtained using just 7 bands that are considerably wider?
- 3. How can this whole wavelength range be covered?

From the information we have now, we will not consider using ADAM, the baseline has been described in section 6.

7 Other a priori data

7.1 Ozone profile shape

For O₃ retrievals (both total column and profile), a total ozone-classified a priori vertical profile climatology is required. The TOMS v8 database by McPeters *et al.* [RD42] provides monthly zonal average ozone profiles for

10° latitude bands with such a classification and is available on the TOMS ftp web site. A new version of this climatology has been recently released [RD43] but no total ozone classification is provided yet. If the latter is distributed in a near-future, it could be tested as an alternative.

To account for the longitudinal variations of the tropospheric ozone content, the tropospheric ozone column climatology from OMI/MLS is used (Ziemke *et al.* [RD44]). This climatology provides monthly mean tropospheric columns with a spatial resolution of $1^{\circ} \times 1.25^{\circ}$ (latitude × longitude) for latitudes ranging between -60° and $+60^{\circ}$. This database is available at [ER6].

7.2 SO₂ profile shape

The baseline for SO_2 retrieval is to use CTM profile shapes, resulting in more realistic profiles from anthropogenic emissions than the box profiles previously assumed. Details are provided in the SO_2 ATBD [RD45, section 5.4.3]. The proposed approach is similar as for the HCHO algorithm: use daily forecast of TM5 or if the forecast is not available a climatological set of profiles from the TM5 or IMAGES models.

7.3 HCHO

The baseline for HCHO is to use daily forecasts from TM5 model (dynamic data input). However, climatology of HCHO profiles based on TM5 model simulations will be created, and used as a backup solution for NRT processing. This database will also be used for the reference sector correction.

- $1^{\circ} \times 1^{\circ}$ in latitude and longitude.
- Monthly profiles at S5P equator crossing time (early afternoon).
- Altitude-grid of the TM5 model (same as for tropospheric NO₂ retrievals).

8 Instrument key data

This item contains data that describes the instruments response to radiation. The most important component of the instrument key data is the spectral slit function, but it may include other data. This data will be generated during the on-ground calibration phase, and may be updated with in-flight observations. Providing this data is the responsibility of the calibration team; the responsibility for updating it lies with the in-flight calibration team.

Items that the level 2 retrieval algorithms need in the instrument key data include:

Instrument slit function Slit function per band and binned spectrum as a function of wavelength

Point spread function Instantaneous 2D shape of each detector pixel within O₂ A-band and SWIR channel.