Overview of Sentinel 5 Precursor Trace Gas, UV, Cloud and Aerosol Products

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TROPOMI L2 PRODUCTS

L2 Working Group

PROTOTYPE

VERIFICATION

PROCESSOR

GOME • SCIAMACHY • OMI • GOME-2

KNMI | DLR | IUP-UB | BIRA | SRON | MPIC | RAL
## Sentinel 5 Precursor – Level 2 Products

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Data Product</th>
<th>Vertical Resolution</th>
<th>Accuracy</th>
<th>Precision</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ozone</td>
<td>Ozone Profile</td>
<td>6 km</td>
<td>10-30%</td>
<td>10%</td>
</tr>
<tr>
<td></td>
<td>Total Ozone</td>
<td>total column</td>
<td>3.5-5%</td>
<td>1.6-2.5%</td>
</tr>
<tr>
<td></td>
<td>Tropospheric Ozone</td>
<td>trop column</td>
<td></td>
<td></td>
</tr>
<tr>
<td>NO₂</td>
<td>Stratospheric NO₂</td>
<td>strat column</td>
<td>&lt; 10%</td>
<td>0.5e15</td>
</tr>
<tr>
<td></td>
<td>Tropospheric NO₂</td>
<td>trop column</td>
<td>25-50%</td>
<td>0.7e15</td>
</tr>
<tr>
<td>SO₂</td>
<td>SO₂ enhanced</td>
<td>total column</td>
<td>30%</td>
<td>0.15-0.3 DU</td>
</tr>
<tr>
<td></td>
<td>Total SO₂</td>
<td>total column</td>
<td>30-50%</td>
<td>1-3 DU</td>
</tr>
<tr>
<td>Formaldehyde</td>
<td>Total HCHO</td>
<td>total column</td>
<td>40-80%</td>
<td>1.2e16</td>
</tr>
<tr>
<td>CO</td>
<td>Total CO</td>
<td>total column</td>
<td>15%</td>
<td>&lt; 10%</td>
</tr>
<tr>
<td>Methane</td>
<td>Total CH₄ (offline)</td>
<td>total column</td>
<td>1.5%</td>
<td>1%</td>
</tr>
<tr>
<td></td>
<td>Cloud Fraction</td>
<td>total column</td>
<td>&lt; 20%</td>
<td>0.05</td>
</tr>
<tr>
<td></td>
<td>Optical Thickness</td>
<td>total</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Product Coordinator</td>
<td>Algorithm Prototype</td>
<td>Independent Verification</td>
<td>Operational Processor</td>
<td></td>
</tr>
<tr>
<td>---------------------</td>
<td>---------------------</td>
<td>--------------------------</td>
<td>-----------------------</td>
<td></td>
</tr>
<tr>
<td>KNMI</td>
<td>IUP</td>
<td>DLR-IMF</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Sentinel 5 Precursor – Level 2 Products (2)**
O$_3$ Total Column – DOAS_NRT (DLR/BIRA)

- Two steps DOAS approach
  - DOAS fit for ozone slant column and effective temperature
  - Iterative AMF/VCD computation using a single wavelength

- Improved O$_3$ Retrieval
  - Molecular Ring correction (Van Roozendael et al., JGR 2006)
  - On-the-fly RTM simulations LIDORT v3.x (Spurr, 2003)
  - Cloud correction using OCRA&ROCINN v3.0 (Loyola et al., TGRS 2007)
  - Adaption to SCIAMACHY (Lerot et al., AMT 2009)
  - Intra-cloud, sun-glint and scan angle corrections (Loyola et al., JGR 2011, Hao et al., 2014)
O$_3$ Total Column – GODFIT_OFL (BIRA/DLR)

- **Direct-Fitting algorithm** (one step retrieval, more accurate than DOAS)
- **RT model**: LIDORT
- **Fitting window**: 325-335 nm
- **A-priori O$_3$ profiles:**
  - Stratosphere: Total column classified climatology TOMSv8
  - Troposphere: OMI/MLS climatology.
- **State vector**: Total Ozone + Effective temperature + effective albedo + Ring
- **Capability for fast processing** using radiance LUTs.
- Baseline Algorithm for generating the CCI total O$_3$ data sets (www.esa-ozone-cci.org).
- Successfully applied to the GOME, SCIAMACHY, GOME-2A/B and OMI sensors.

*See also posters of C. Lerot et al.; M. Koukouli et al. Lerot et al., JGR, 2014.*
Ozone Profile (incl. troposphere) Algorithm (KNMI)

- 3D view on ozone
- Vertical resolution: ~6 km (sampling 20 levels)
- Horizontal resolution: 21x28 km² (7x7 km²)
- *Tropospheric column are strongly affected by a-priori*
- *Tropospheric averaging kernels show significant contributions from the stratosphere*
- Heritage: OMI/GOME-2/GOME

One orbit of OMO3PR profile data in VMR. The image on top: total column ozone in DU.
Ozone Profile Verification (RAL, IUP-UB)

Two different scientific algorithms:
1. RAL Ozone Profile Algorithm (Munro et al., 1998, Miles et al., 2015)
2. IUP Ozone Profile Retrieval (based on Hoogen et al., 1999)

Verification approach:
1) RTM simulation
2) Linear simulations (error mapping) from simulated profiles
3) Non-linear, fully iterative retrievals from simulated radiances
4) Comparison of retrieval diagnostics
5) Comparison of retrievals using real data

Linear error mapping from simulated profiles (IUP Bremen):

Non-linear, iterative retrieval simulations (RAL)
Typical comparison for GOME-2 CCD to sondes
- Slight offset ~2 DU (CCD is higher)
- Good agreement with annual cycle

Comparsion to SCIAMACHY (limb-nadir matching)
- Offset of 20% added to GOME_CCD data to correct for different altitude ranges:
  SCIA 0-16 km
  CCD 0-10 km
- Difference SCIA-CCD ~2 DU (CCD is lower)
Tropospheric Ozone Algorithm – CSA (IUP-UB)

a) Cloud top heights

b) SCIAMACHY CSA upper tropospheric ozone (Summer) 2003-2011

[Map showing cloud top heights and ozone concentrations across different regions.

Ozone VMR [ppbv]

2003 2004 2005 2006 2007 2008 2009 2010 2011]
Tropospheric Ozone Verification (IUP-UB)

Table 1: Station Mean Comparison

<table>
<thead>
<tr>
<th>Station</th>
<th>Prot Mean (DU)</th>
<th>Ver Mean (DU)</th>
<th>Sondes Mean (DU)</th>
<th>R Ver VS Sondes</th>
<th>R Prot VS Sondes</th>
<th>R Prot VS Ver</th>
</tr>
</thead>
<tbody>
<tr>
<td>Natal</td>
<td>27.8</td>
<td>28.1</td>
<td>28.9</td>
<td>0.83</td>
<td>0.91</td>
<td>0.91</td>
</tr>
<tr>
<td>Java</td>
<td>18.8</td>
<td>18.6</td>
<td>21.5</td>
<td>0.48</td>
<td>0.60</td>
<td>0.69</td>
</tr>
</tbody>
</table>

Mean difference: 1.5 DU

where used as test data.
The Dutch OMI NO$_2$ (DOMINO) processing system is the basis for the TROPOMI NO$_2$ data product, based on a DOAS retrieval and an estimate of the stratospheric NO$_2$ column and tropospheric profiles from a data assimilation / chemistry transport model system.

Updates w.r.t. current OMI processing:
- Improved slant column retrieval
- Upgraded CTM from TM4 at 3° × 2° to TM5 at 1° × 1° with CB05 chemistry scheme and updated emissions
- Updated stratospheric NO$_2$ assimilation scheme
- Improved description of terrain height and clouds
NO$_2$ Total and Tropospheric Verification (IUP-UB, MPIC, DLR)

- NO$_2$ Slant columns
- NO$_2$ stratospheric correction
- NO$_2$ AMF

Differences in trop NO$_2$ residues for different stratospheric corrections (prototype - verification) for OMI

01.2005

07.2005

Correlation of OMI NO$_2$ SCs from prototype and verification algorithm

Same settings

Free settings

Comparison between BAMFs from different models

Very good consistency found, problems fixed, work ongoing (AMFs for different inputs)
SO₂ Algorithm (BIRA)

- **3-steps DOAS algorithm**
  - Spectral fitting in multiple windows to avoid saturation
    - 312-326 nm (pollution, volcanic degassing)
    - 325-335 nm (moderate eruptions)
    - 360-390 nm (extreme eruptions)
  - Background correction and destriping
  - Air mass factor calculation using modeled (anthropogenic SO₂) and predefined profiles (volcanic SO₂) + error analysis and averaging kernels calculation.

- **Prototype algorithm applied to synthetic spectra**

- **Prototype algorithm extensively tested on OMI data (10 years) and compared to ground-based and other satellite datasets** (Theys et al., JGR, 2015)

  See also talk of N. Theys
SO₂ Verification (MPIC, DLR)

• **Similar to Prototype:**
  
  3-steps DOAS algorithm, but different fit windows
  
  312-324 nm (312-326, degassing)
  
  318-335 nm (325-335, moderate eruptions)
  
  323-335 nm (360-390, major eruptions)

• **Extensive intercomparison between Prototype and Verification Algorithm for various synthetic scenarios (SO₂ VCDs and profiles, geometries)**

  → general good agreement, but inconsistencies possible depending on fit window transition criteria

  → Verification Algorithm tries to guarantee smooth transition by mixing results from fit windows

• **Fit window transition criteria based on synthetic spectra simulating volcanic eruptions**
HCHO Algorithm (BIRA)

Formaldehyde as a Tracer of Hydrocarbon Emissions

- TROPOMI ATBD based on BIRA-IASB OMI HCHO product (De Smedt et al., 2015).
- The 7x7 km² spatial resolution of TROPOMI, combined with a SNR equivalent (or even better) than OMI, is expected to significantly improve the HCHO observations.
HCHO Verification (IUP-UB)

- HCHO Slant columns
- HCHO offset corrections
- HCHO AMF

⇒ Very good consistency found if settings are the same
⇒ Large sensitivity to settings and background used
⇒ problems identified and fixed,
⇒ work ongoing (AMFs, …)
# CO Algorithm – SICOR (SRON)

<table>
<thead>
<tr>
<th>Approach</th>
<th>Full-physics</th>
</tr>
</thead>
</table>
| Data coverage  | Ocean and land  
|                | Clear-sky and cloud |
| Performance    | 0.15 sec / retrieval  
|                | Precision < 10%  
|                | Accuracy ~ 4% |

**Results for synthetic ensemble**

**Results for SCIAMACHY**
CO Verification – BESD (IUP-UB)

- Bremen Optimal Estimation DOAS
- Heritage: XCO$_2$ retrieval from SCIAMACHY (Reuter et al., 2010, 2011) and GOSAT (Heymann et al., 2015)
- Full Physics
- Developed to consider scattering at optically thin cirrus and aerosol
- Using complete S-5P Bands 6-8 (NIR-SWIR)

Findings:
- SICOR performs very well within the requirements: required: < 10%
- Required: < 8%

Scenarios compared between prototype and verification algorithm:
- Varying albedo, aerosols, clouds, solar zenith angles, ...
- Findings:
  - SICOR performs very well within the requirements
**CH4 Algorithm – RemoTeC (SRON)**

<table>
<thead>
<tr>
<th>Approach</th>
<th>Full-physics</th>
</tr>
</thead>
<tbody>
<tr>
<td>Data coverage</td>
<td>Land and sun-glint</td>
</tr>
<tr>
<td></td>
<td>Clear-sky</td>
</tr>
<tr>
<td>Performance</td>
<td>10 sec / retrieval</td>
</tr>
<tr>
<td></td>
<td>Precision ~ 0.35%</td>
</tr>
<tr>
<td></td>
<td>Accuracy ~ 0.47%</td>
</tr>
</tbody>
</table>

Results for synthetic ensemble

Results for GOSAT
CH4 Verification – BESD (IUP-UB)

• Same algorithm as for CO verification

- Scenarios compared between prototype and verification algorithm:
  - Spectrally varying albedo, aerosols, clouds, solar zenith angles, ...
- Findings:
  - RemoTeC performs very well within the requirements

required: < 0.6%

required: < 0.8%
Clouds Algorithm – OCRA & ROCINN (DLR)

GOME type

O2 A-Band

ROCINN (CRB+CAL)

UVN

OCRA

\[ c_f = \sqrt{\sum_{i=R,G,B} \alpha(\lambda_i) \max(0, [\rho(\lambda_i) - \rho_{CF}(\lambda_i)]^2 - \beta(\lambda_i))} \]

Optical thickness

Cloud-top height

Cloud fraction
Clouds Verification (IUP-UB, KNMI)

Y-axis: **ROCINN-CRB** (Lambertian cloud)
X-axis: **SACURA** (scattering cloud)

Cloud height bias: SACURA - ROCINN

Main sources of difference

(1) **Multi-layered clouds**
(2) **Surface climatology**
(3) **Cloud model**

![Chart showing the relationship between SACURA and ROCINN with main sources of difference highlighted.

R = 0.889, y = 0.696x + 0.490

R = 0.635, y = 0.522x + 2.067

Labels: (1) WATER, (2) LAND, (3) Other areas.
Aerosols Index Algorithm (KNMI)

- UVAI is a derived (not retrieved) quantity with fixed definition
  - Not much room for algorithm changes

- Prototype algorithm strongly based on operational algorithm (KNMI)
- Wavelength pairs: 340/380 and 354/388 nm
- Auxiliary input:
  - Ozone total column from ECMWF 3h-forecast (for NRT UVAI)
  - Mean surface altitude from digital elevation map (GMTED2010, USGS)
- LUT calculation as for operational algorithm (Tilstra et al. JGR 2012) with DISAMAR

- Verification algorithm very similar to prototype and operational algorithms
- Wavelength pairs: 340/380 and 354/388 nm
- Auxiliary input:
  - Ozone total column from operational TROPOMI product
  - Mean surface pressure from digital elevation map (DEM, NASA)
- LUT calculation as for operational algorithm (Tilstra et al. JGR 2012) with McArtim3
Aerosols Index Verification (MPIC)

- Study agreement between algorithms: “truth” is not known (unlike, e.g. for gases)
- Tests with synthetic data
- Comparison of GOME-2 results from operational, prototype, and verification algorithm (Aug. 13, 2007)
  - Qualitative agreement good; more detailed comparison in progress
    - Offset
    - Viewing angle-dependent diff.
Aerosols Layer Height Algorithm (KNMI)

Newly developed ALH-algorithms, both based on O$_2$ absorption: O$_2$ A-band around 760 nm with strong and weak lines

Prototype:
- Spectral fit (DISAMAR) of reflectances 758-770 nm
- Aerosol model: H-G with $g = 0.7$ and SSA = 0.95
- Profile parameterization: elevated scattering layer with an assumed geometric thickness
- 2-parameter retrieval: AOT and aerosol layer height

Verification
- Optimal estimation algorithm (SCIATRAN)
- Profile parameterization: scattering layer starting at surface
- 2-parameter retrieval: AOT and aerosol layer top height
- Aerosol models from AERONET climatology
- Retrieval using on LUT-based weighting functions
Aerosols Layer Height Verification (IUP-UB)

- Ash plume from Eyjafjallajökull volcano 2010
- Comparison of verification algorithm results (GOME-2 and MERIS) and prototype algorithm (GOME-2) with MISR (“truth”)
UV* Algorithm (FMI)

- UV radiation has a broad range of effects concerning life on Earth:
  - human health
  - longevity of materials
  - climate and air quality
  - ecosystems: plants, animals

- UV algorithm and input data:
  - LIDORT radiative transfer model to produce relevant look-up-tables
  - total ozone column as measured/retrieved by TROPOMI
  - reflectance at 354 nm from TROPOMI to determine the cloud optical thickness
  - climatologies of surface albedo and atmospheric aerosol load

- UV Product:
  - near-global coverage of surface UV and daily doses
  - needed (also) to continue TOMS & OMI UV heritage
S5P L2 Processors – PDGS Context

Chart 29

DRL / Inuvik Receiving Station
KSAT/Svalbard Receiving Station

Uninett Nordnet

GÉANT

CANARIE

KNMI

Aux Data Provider

Flight Operation Segment

Expert Teams

External Users

GMES Service MACC

Internet

Firewall

ESTEC Data Pool

Copernicus WAN

other Sentinel PACs and CGSs

Frankfurt

Sentinel Data Hub Firewall

Sentinel Data Hub

Sentinel Firewall

Sentinel OP Firewall

S1/S3(S5p) PAC

DMZ Core Sw.

S5p DMZ

Access Switch

S5p "ODA"

DLR Firewall

2*1 Gbit/s

DLR public DMZ

1 Gbit/s

DLR protected DMZ

2*1 Gbit/s

2*500 Mbit/s

Router/Switch

2*1 Gbit/s

DLR EOC

EOC OP Firewall

S5p Production VLAN, 1 Gbit/s

Sentinel LTA Firewall

Intern Core Sw.

10 Gbit/s

DMZ Core Sw.

8 Gbit/s

FC SAN

10 Gbit/s

Transfer Zone

Del. Disk

ECCS Processing and Archiving Environment

S5p Archive Server

S5p L0 Processing Servers

S5p L1 NRT Proc. Servers

S5p L2 NRT Proc. Servers

S5p L1 Off. Proc. Servers

S5p L2 Off. Proc. Servers

S5p Internal Dissemination Server

S5p Interface Server
S5P L2 Processors – Big Data Challenger

S5P smaller pixels and larger swath-width
- more than 1 million pixels/orbit
- 80 minutes/orbit, just under 5 ms/pixel
  - Processors are multi-threaded
  - Pixel selection is applied where needed

Compared to GOME & OMI:
- increase in spectral range
  - L1B ~ 35 GB/orbit
S5P L2 Processors – File Format

- One file per product
- Common netCDF structure
- netCDF-4 library available for almost all data analysis environments and most common programming languages
- The netCDF file format is self-describing
- Metadata is contained within the main group
- NetCDF-4 uses an enhanced version of HDF-5 as the storage layer
  - any HDF-5 applications can read the S5P L2 products.

For more details see poster #53 from Sneep et al.
S5P L2 Processors – File Format (2)

cloud_optical_thickness

cloud_top_height

cloud_top_height ()

Data Min = 0.0, Max = 15.0, Mean = 3.4