sentinel-5p

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

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ATMOS, Heraklion, 11-JUN-2015

DLR
SRON
MAX-PLANCK-INSTITUT FÜR CHEMIE
iup
RAL Space
FMI

TROPOMI L2 PRODUCTS

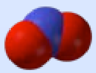
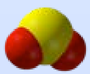
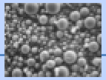
L2 Working Group

PROTOTYPE | VERIFICATION | PROCESSOR

GOME ◦ SCIAMACHY ◦ OMI ◦ GOME-2

KNMI | DLR | IUP-UB | BIRA | SRON | MPIC | RAL

Sentinel 5 Precursor – Level 2 Products

Parameter	Data Product	Vertical Resolution	Accuracy	Precision
Ozone  	Ozone Profile	6 km	10-30%	10%
	Total Ozone	total column	3.5-5%	1.6-2.5%
	Tropospheric Ozone	trop column		
NO_2 	Stratospheric NO_2	strat column	< 10%	0.5e15
	Tropospheric NO_2	trop column	25-50%	0.7e15
SO_2  	SO_2 enhanced	total column	30%	0.15-0.3 DU
	Total SO_2	total column	30-50%	1-3 DU
Formaldehyde 	Total HCHO	total column	40-80%	1.2e16
CO	Total CO	total column	15%	< 10%
Methane 	Total CH_4 **(offline)**	total column	1.5%	1%
	Cloud Fraction	total column	< 20%	0.05
	Optical Thickness	total		

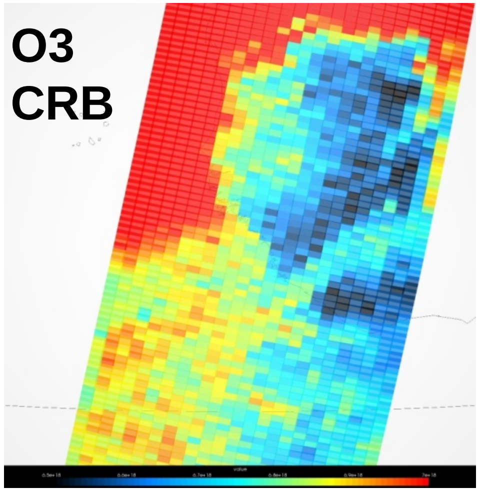
Sentinel 5 Precursor – Level 2 Products (2)

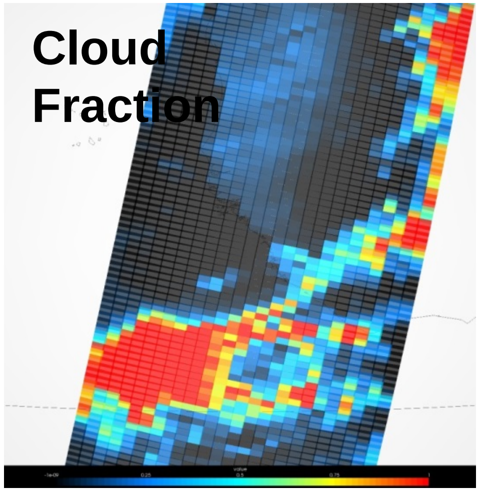
Product	Algorithm Prototype	Independent Verification	Operational Processor
Coordinator	KNMI	IUP	DLR-IMF

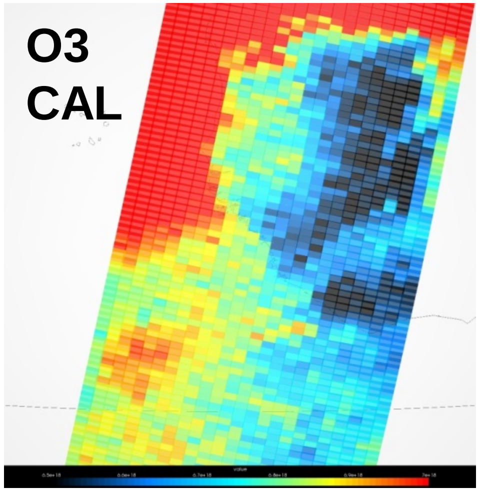
O_3 Total Column – DOAS_NRT (DLR/BIRA)

- Two steps DOAS approach
  - DOAS fit for <u>ozone slant column</u> and <u>effective temperature</u>
  - 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)



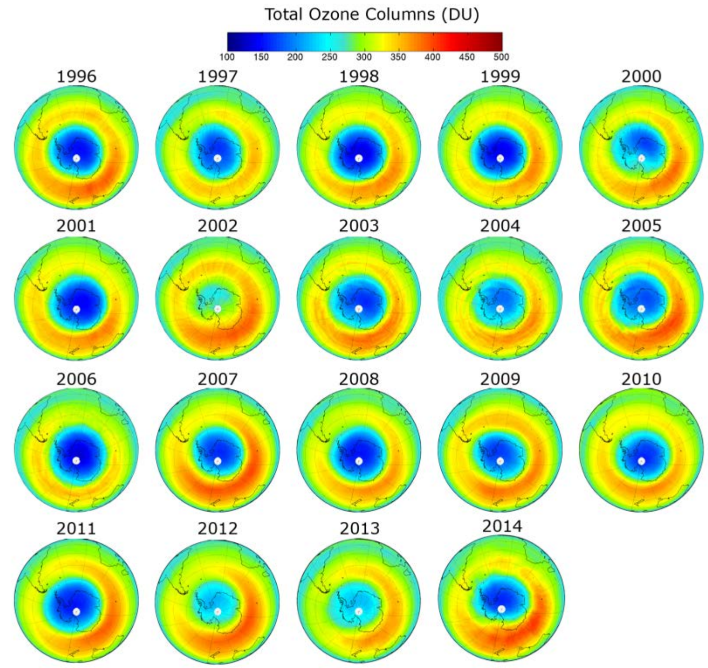


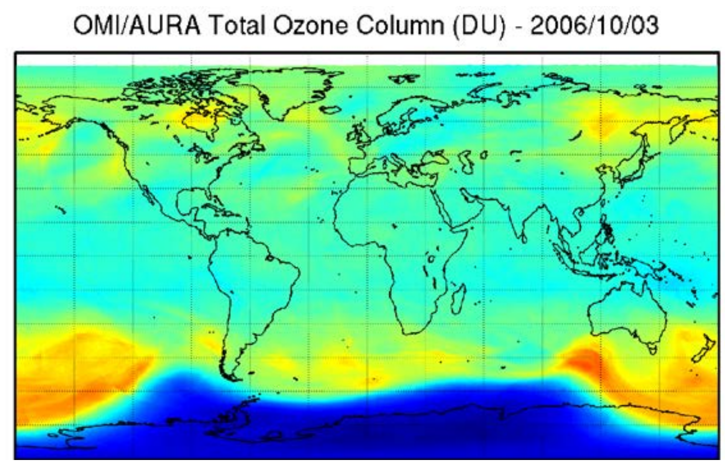


O_3 Total Column – GODFIT_OFL (BIRA/DLR)

- **Direct-Fitting algorithm** (one step retrieval, more accurate than DOAS)
- **RT model:** LIDORT
- **Fitting window:** 325-335 nm
- **A-priori O3 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 O3 data sets (www.esa-ozone-cci.org).
- Successfully applied to the GOME, SCIAMACHY, GOME-2A/B and OMI sensors.

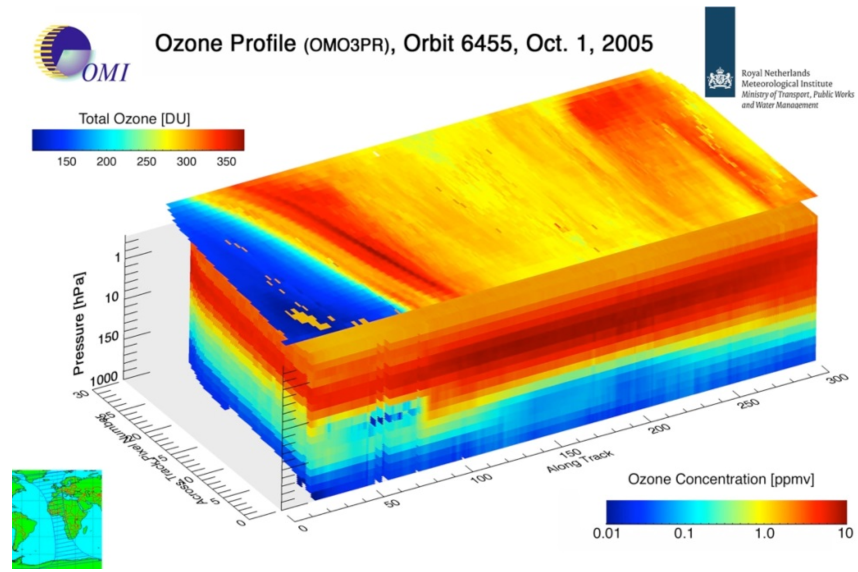
See also posters of C. Lerot et al.; M. Koukouli et al.
Lerot et al., JGR, 2014.



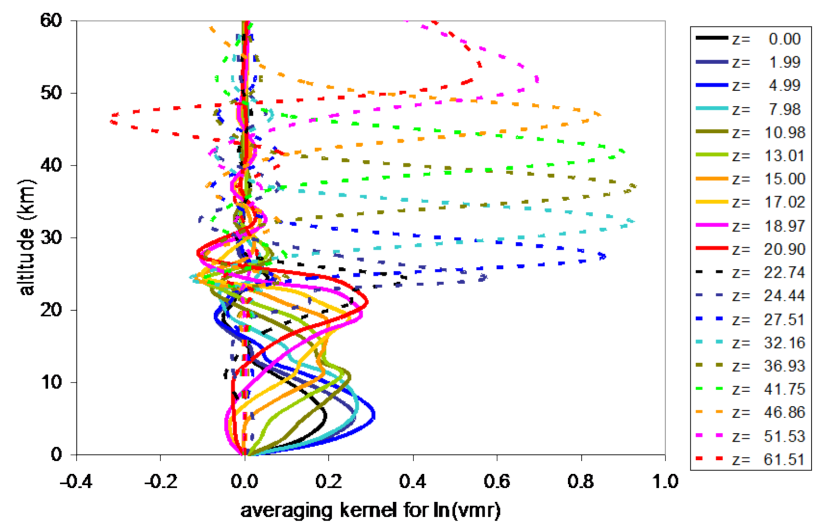


Ozone Profile (incl. troposphere) Algorithm (KNMI)

- 3D view on ozone
- Vertical resolution: ~6 km (sampling 20 levels)
- Horizontal resolution: 21x28 km^2 (7x7 km^2)
- *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.



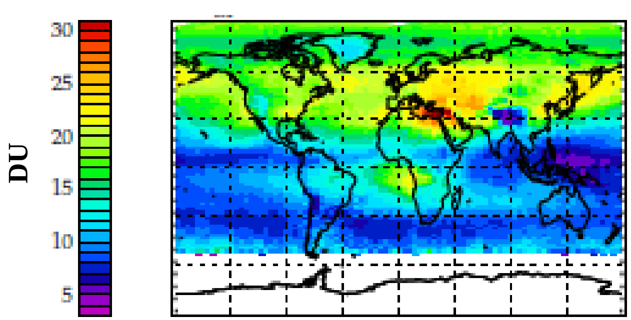
Ozone Profile Verification (RAL, IUP-UB)

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:

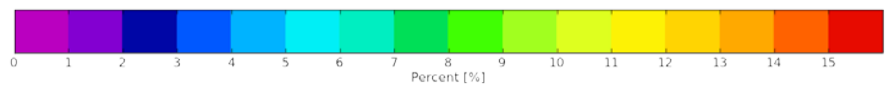
1) RTM simulation
2) Linear simulations (error mapping) from simultated profiles
3) Non-linear, fully iterative retrievals from simulated radiances
4) Comparison of retrieval diagnostics
5) Comparison of retrievals using real data

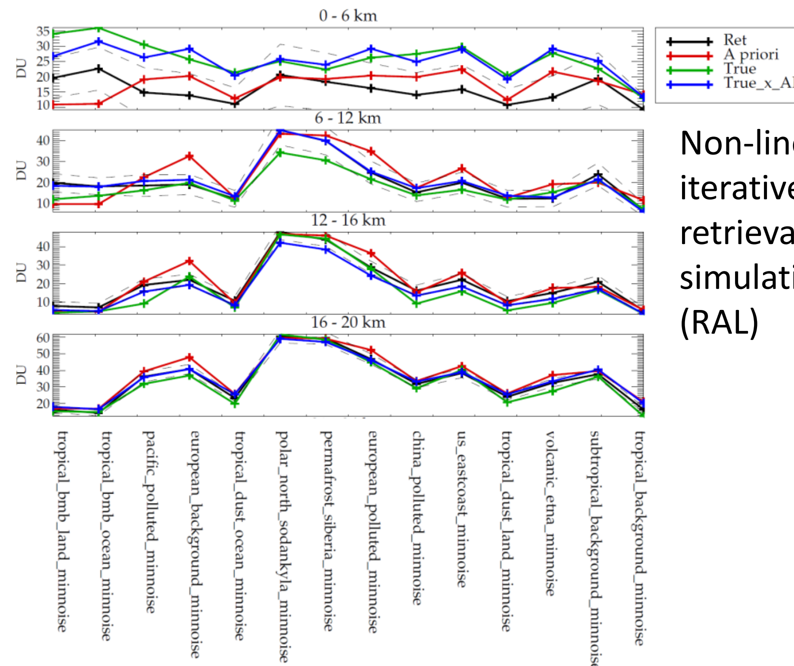


Lower tropospheric ozone July 2008 (RAL)

Linear error mapping from simulated profiles (IUP Bremen):

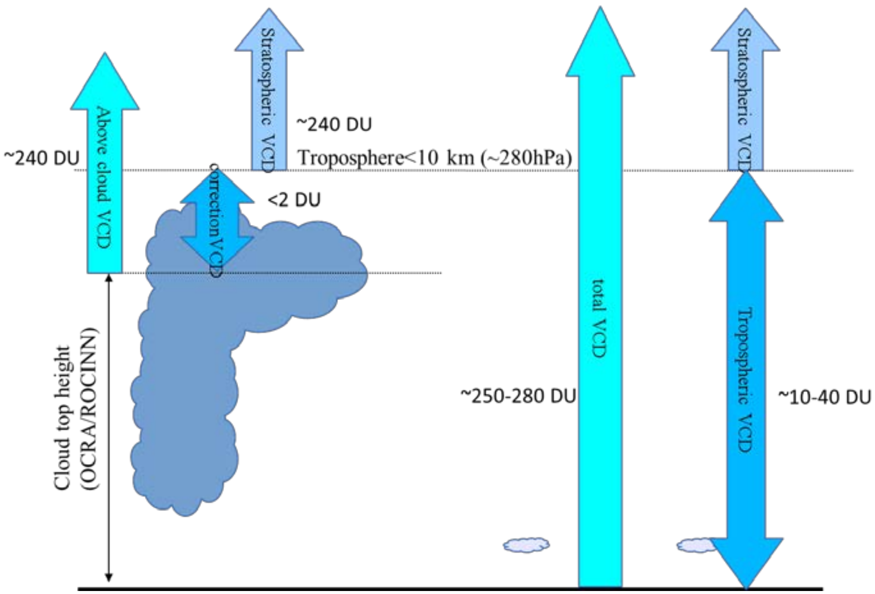
	case1_European_background	case2_European_polluted	case3_China_polluted	case4_Pacific_polluted	Case5_US_Eastcoast	case6_Tropical_background	case7_Tropical_bmb_land	case8_Tropical_bmb_ocean	case9_Tropical_dust_land	case10_Tropical_dust_ocean	case11_Subtropical_Background	case12_Stratospheric_intrusion	case13_Polar_north_sodankyla	case14_Polar_south_marambio	case15_Permafrost_siberia	case16_Volcanic_etna
18 - TOA	0.6	0.2	2.7	3.8	0.1	0.3	3.3	0.01	1.8	2.1	0.8	5.9	2.9	0.6	4.1	1.3
12 - 18 km	0.5	0.2	10.4	5.8	2.3	3.7	7.1	1.4	12.1	6.7	1.0	4.2	3.5	3.2	2.3	6.7
6 - 12 km	0.3	3.7	13.4	12.1	9.9	6.7	13.6	2.5	12.9	8.4	0.2	2.1	4.1	1.1	7.8	13.1
0 - 6 km	1.9	19.1	10.2	9.6	12.5	5.5	13.9	5.9	3.4	2.9	1.2	0.5	21.1	21.2	5.3	7.6

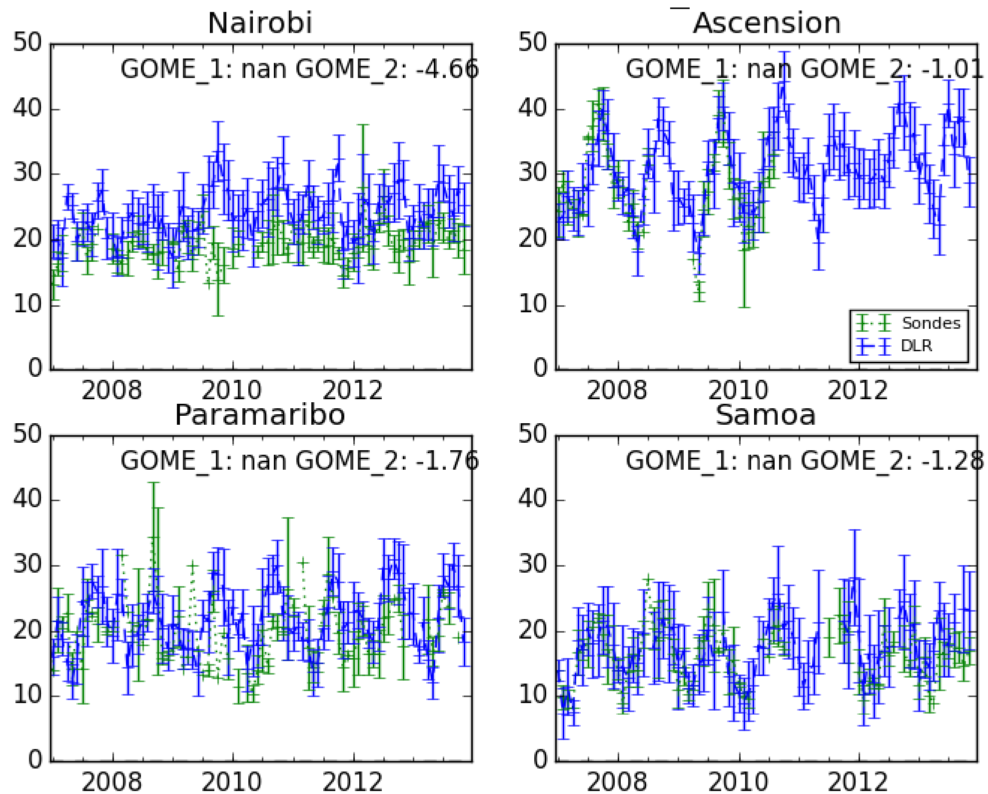




Non-linear, iterative retrieval simulations (RAL)

Tropospheric Ozone Algorithm – CCD (DLR)





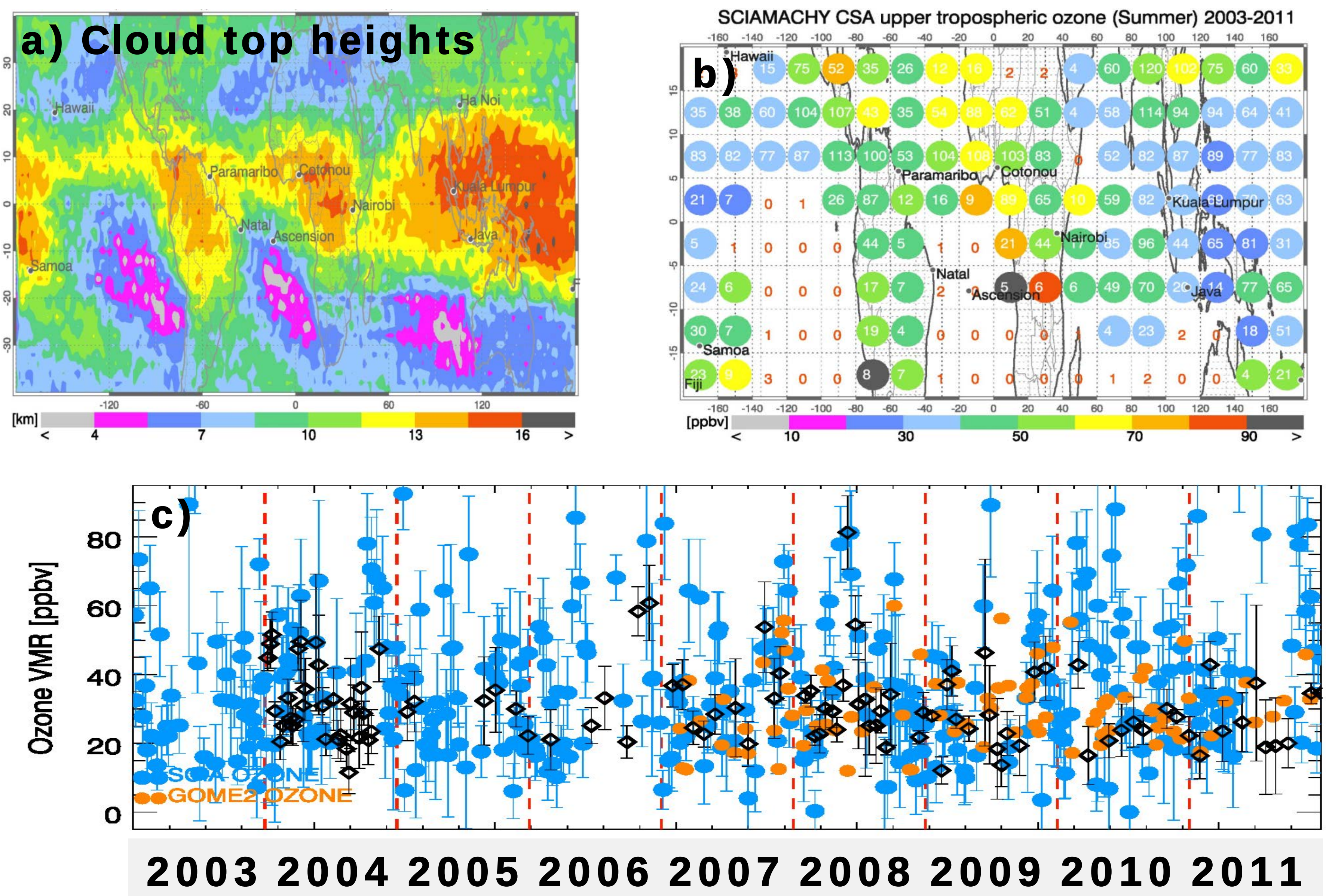
Comparsion to SCIAMACHY (limb-nadir matching)

- 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)

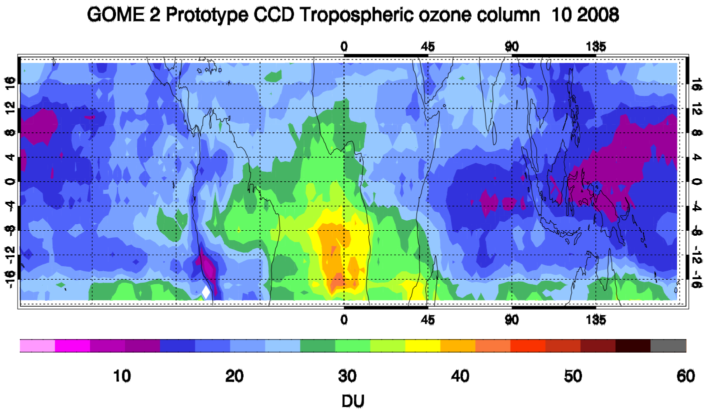
Typical comparison for GOME-2 CCD to sondes

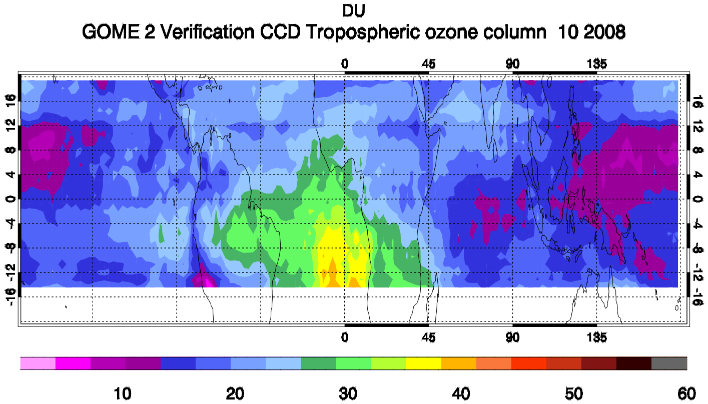
- Slight offset ~2 DU (CCD is higher)
- Good agreement with annual cycle

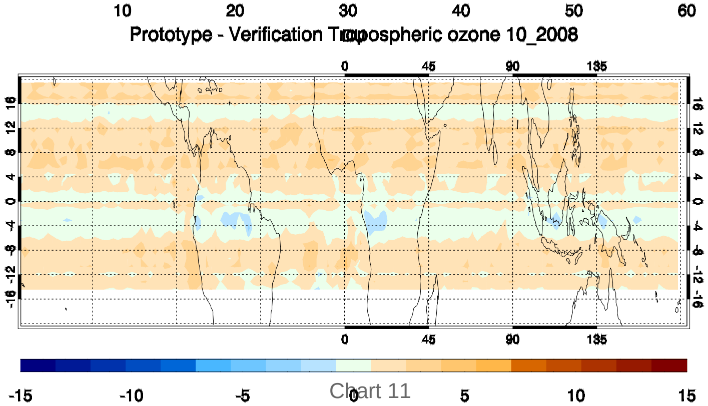
Tropospheric Ozone Algorithm – CSA (IUP-UB)



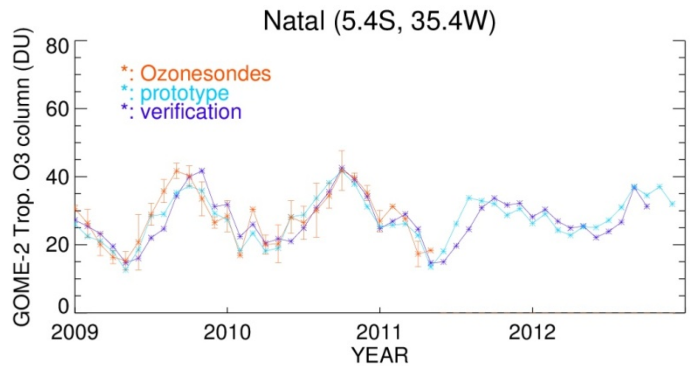
Tropospheric Ozone Verification (IUP-UB)

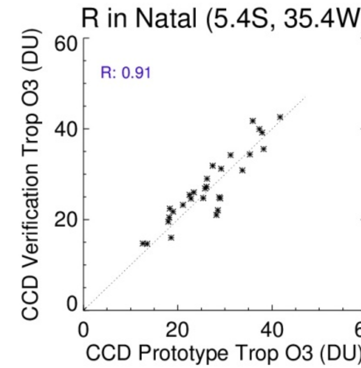


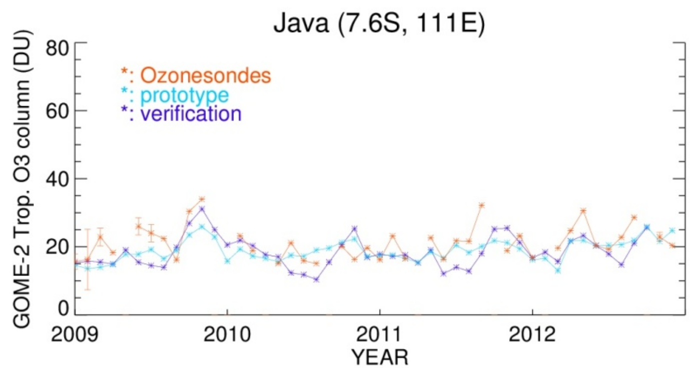


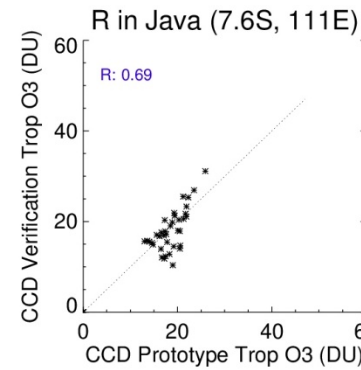


Mean difference: 1.5 DU







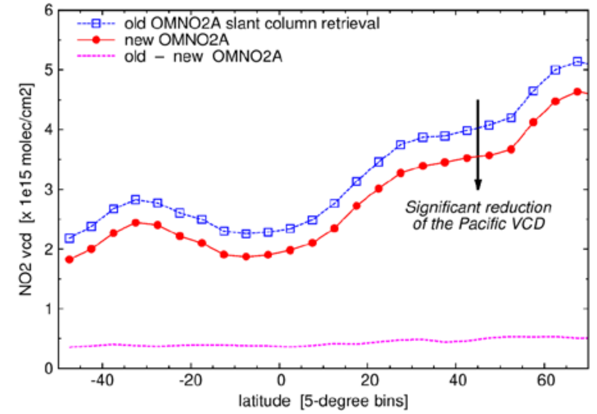


Station	Prot Mean (DU)	Ver Mean (DU)	Sondes Mean (DU)	R Ver VS Sondes	R Prot VS sondes	R Prot VS Ver
Natal	27.8	28.1	28.9	0.83	0.91	0.91
Java	18.8	18.6	21.5	0.48	0.60	0.69

where used as test data.

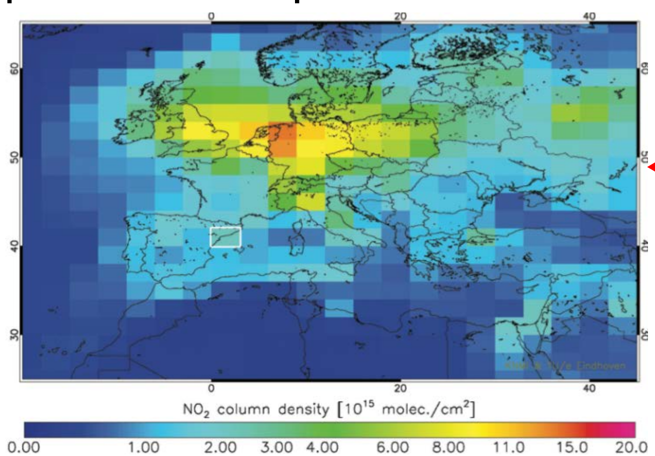
NO_2 Total and Tropospheric Algorithm (KNMI)

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.



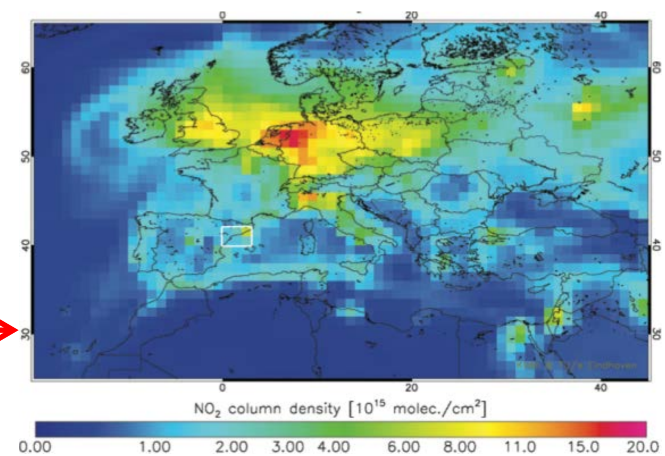
Updates w.r.t. current OMI processing:

- 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



3° × 2°

1° × 1°

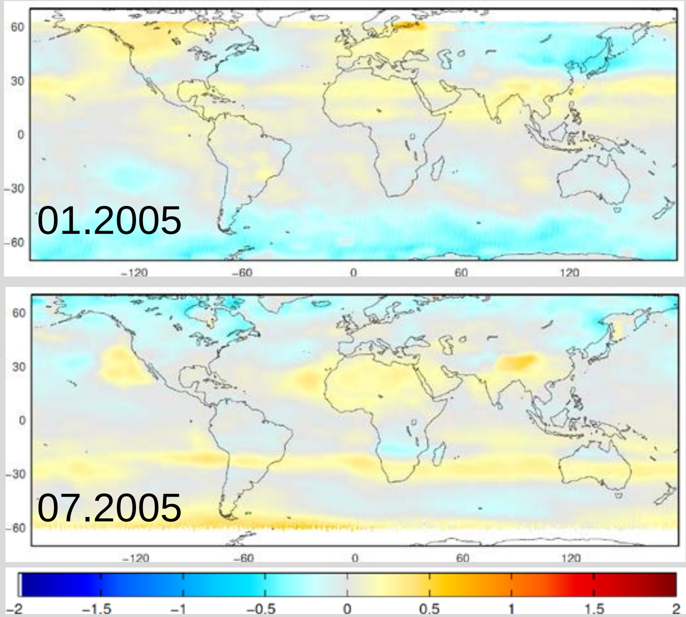


OMI

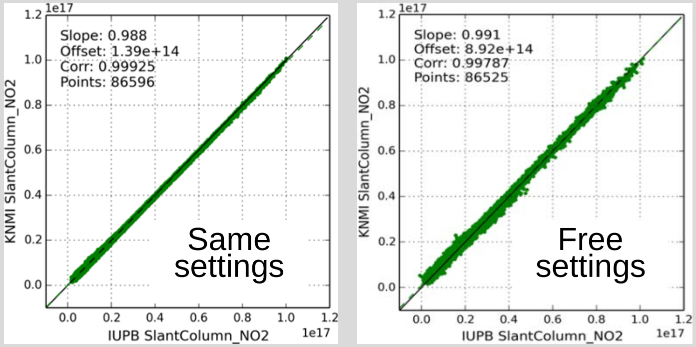
NO_2 Total and Tropospheric Verification (IUP-UB, MPIC, DLR)

- NO_2 Slant columns
- NO_2 stratospheric correction
- NO_2 AMF

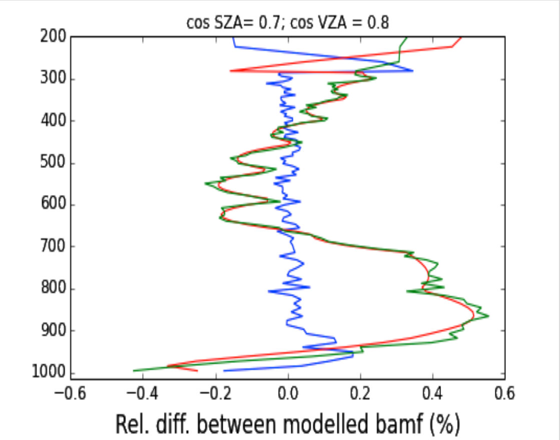
Differences in trop NO_2 residues for different stratospheric corrections (prototype - verification) for OMI



Correlation of OMI NO_2 SCs from prototype and verification algorithm



Comparison between BAMFs from different models

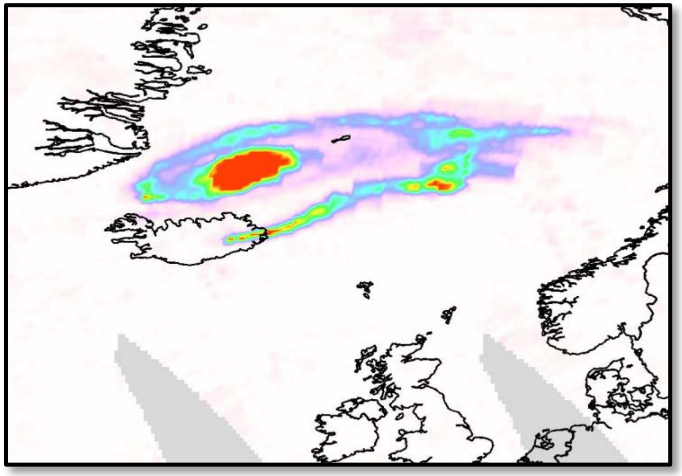


Very good consistency found, problems fixed, work ongoing (AMFs for different inputs)

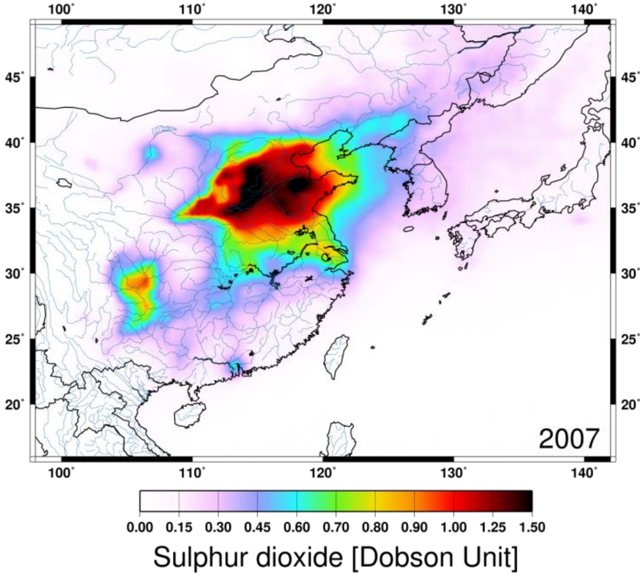
SO_2 Algorithm (BIRA)

- **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 SO_2) and predefined profiles (volcanic SO_2) + 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



SO_2 plume from Holuhraun, 02-09-2014



SO_2 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)

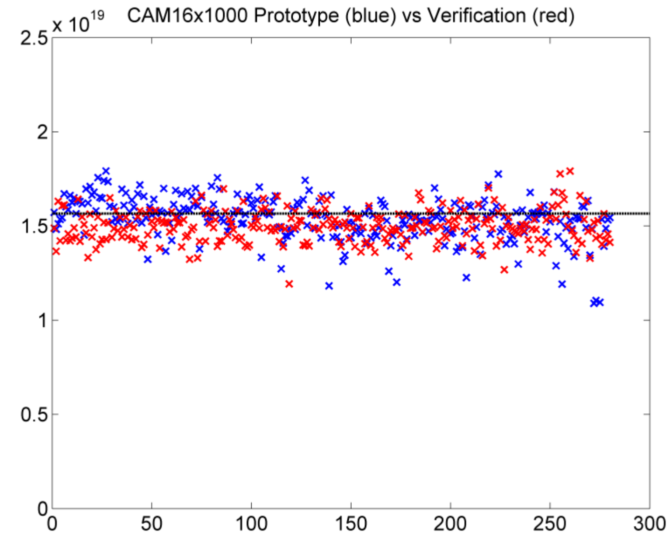
  323-335 nm (360-390, major eruptions)

- **Extensive intercomparison between Prototype and Verification Algorithm for various synthetic scenarios (SO_2 VCDs and profiles, geometries)**

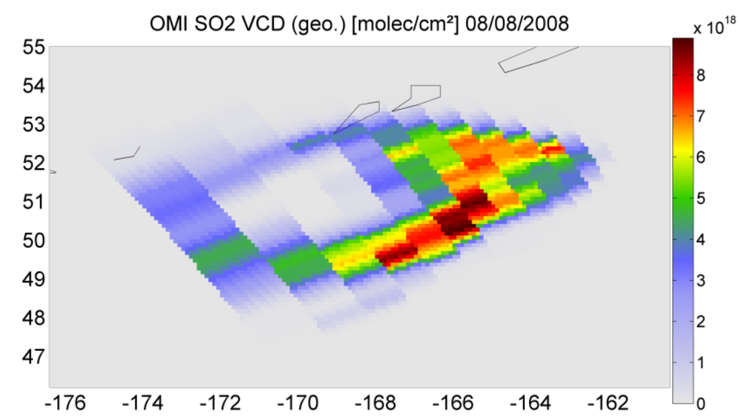
  → general good agreement, but inconsistencies possible depending on fit window transition criteria

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

- **Fit window transition criteria based on synthetic spectra simulating volcanic eruptions**



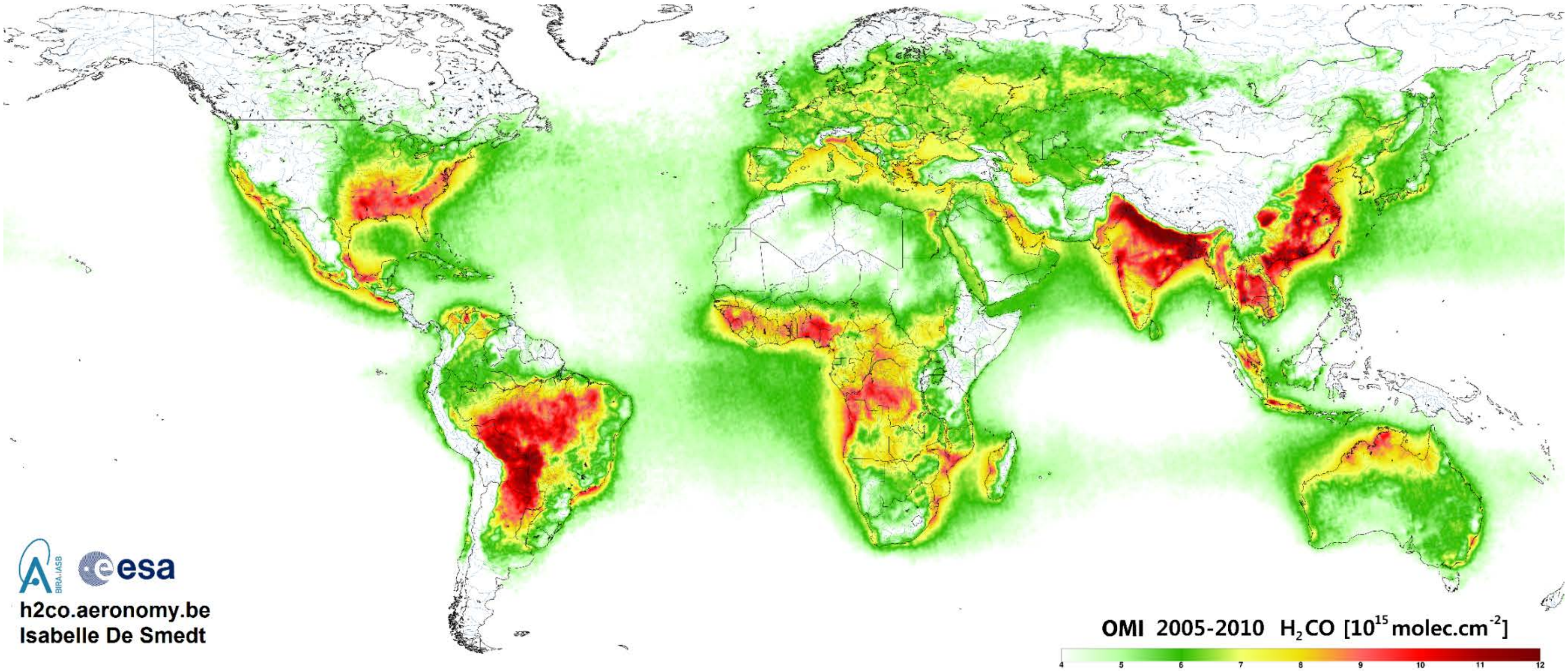
Intercomparison Prototype/Verification for extreme SO_2 VCDs (≈ 600 DU)



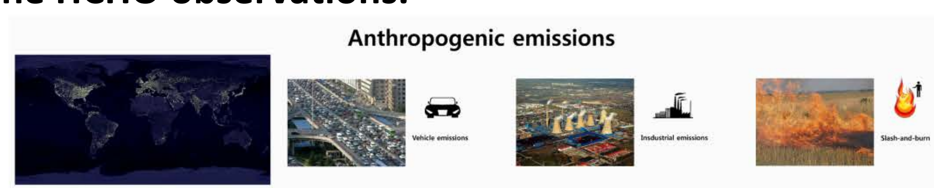
OMI SO_2 plume after Kasatochi eruption on 8th August 2008 (Verification Algorithm)

HCHO Algorithm (BIRA)

Formaldehyde as a Tracer of Hydrocarbon Emissions



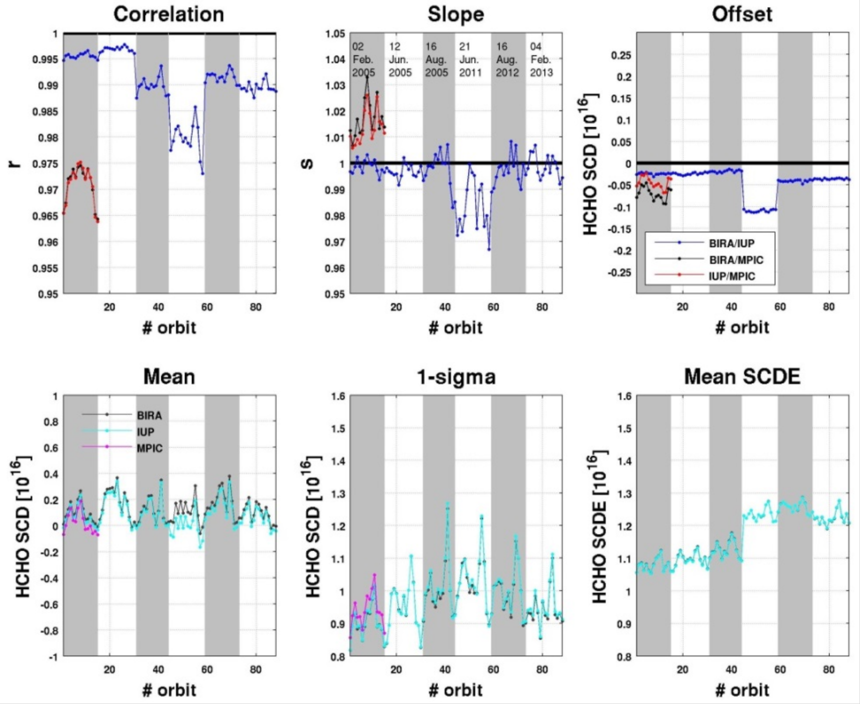
- ✓ **TROPOMI ATBD based on BIRA-IASB OMI HCHO product (De Smedt et al., 2015).**
- ✓ **The 7x7 km^2 spatial resolution of TROPOMI, combined with a SNR equivalent (or even better) than OMI, is expected to significantly improve the HCHO observations.**



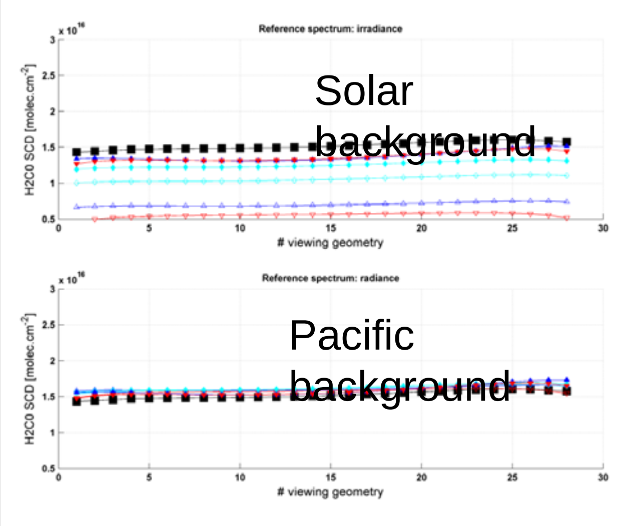
HCHO Verification (IUP-UB)

- HCHO Slant columns
- HCHO offset corrections
- HCHO AMF

HCHO columns using harmonized settings and offset correction for 6 selected OMI days



HCHO columns applying different settings for synthetic spectra using CAMELOT scenarios



⇒ Very good consistency found if settings are the same

⇒ Large sensitivity to settings and background used

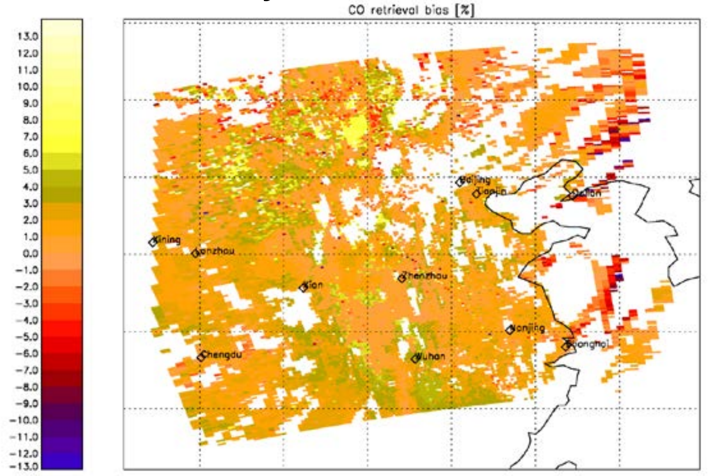
⇒ problems identified and fixed,

⇒ work ongoing (AMFs, …)

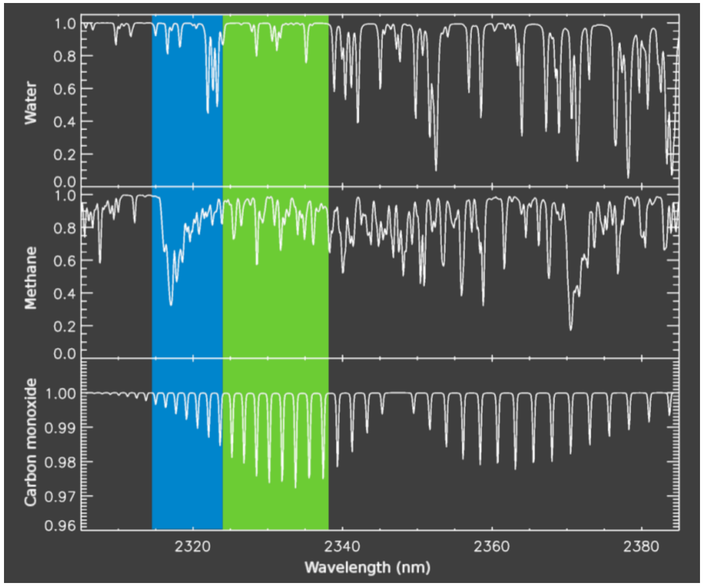
CO Algorithm – SICOR (SRON)

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

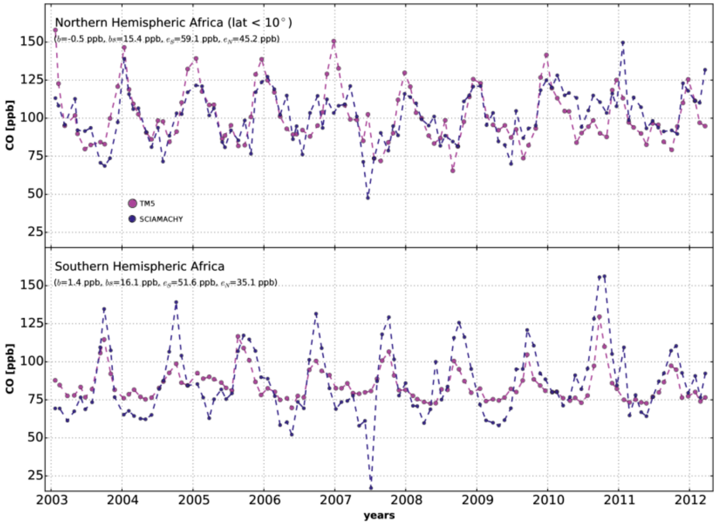
Results for synthetic ensemble



Spectral window



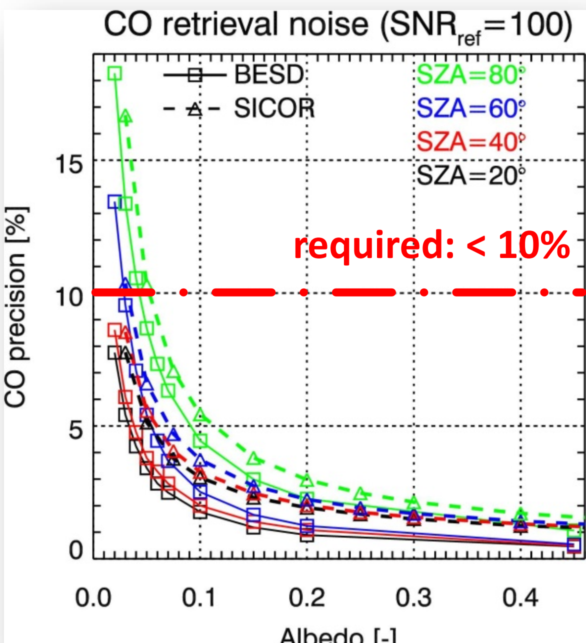
Results for SCIAMACHY

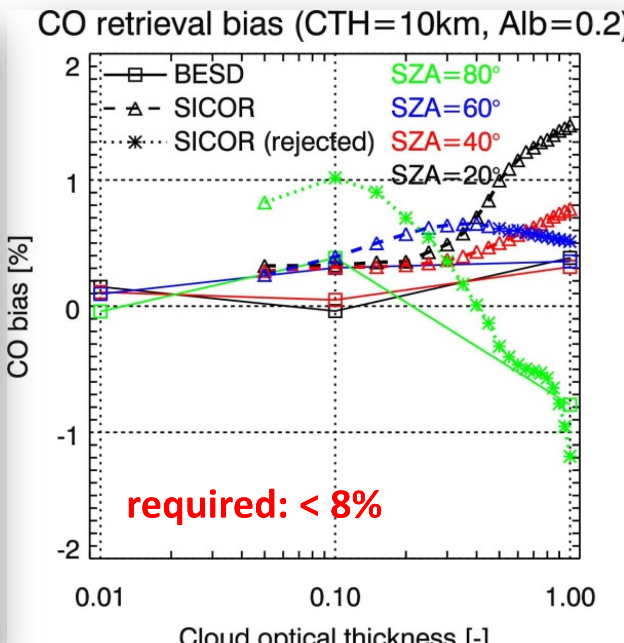


CO Verification – BESD (IUP-UB)

- 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)



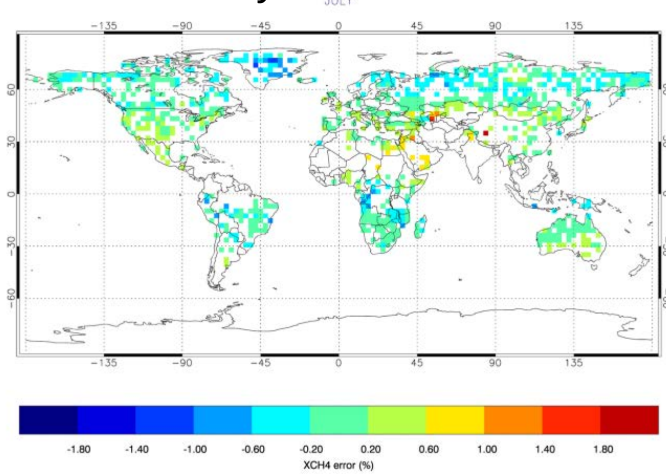


- Scenarios compared between prototype and verification algorithm:
  - Varying albedo, aerosols, clouds, solar zenith angles, …
- Findings:
  - SICOR performs very well within the requirements

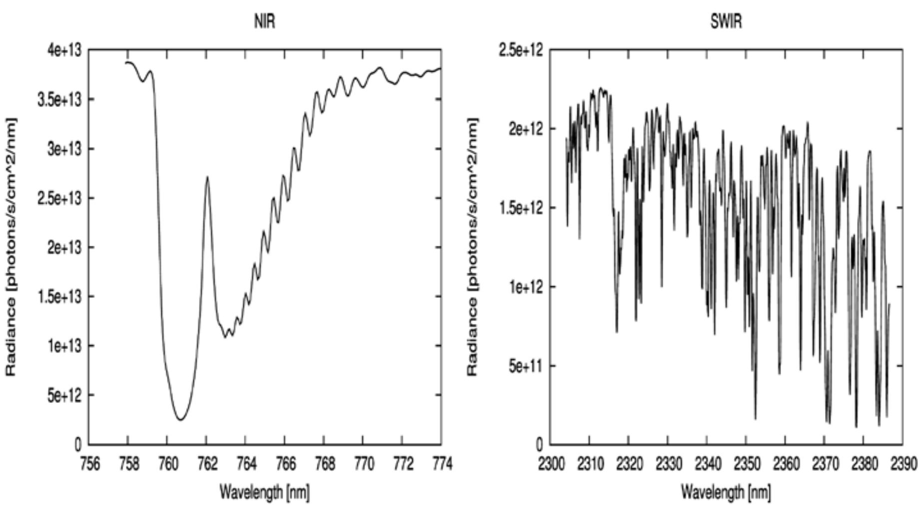
CH4 Algorithm – RemoTeC (SRON)

Approach	Full-physics
Data coverage	Land and sun-glint Clear-sky
Performance	10 sec / retrieval Precision ~ 0.35% Accuracy ~ 0.47%

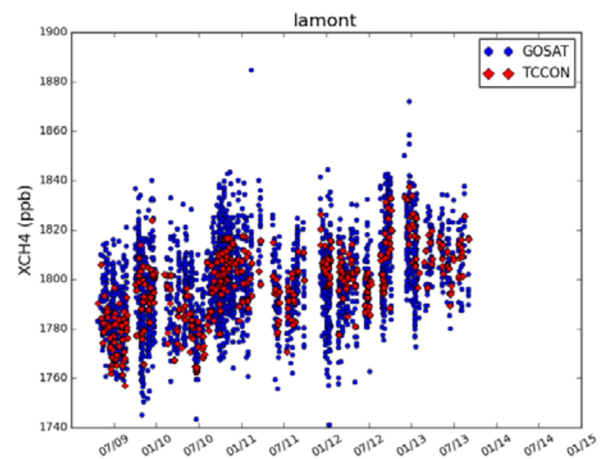
Results for synthetic ensemble



Spectral window

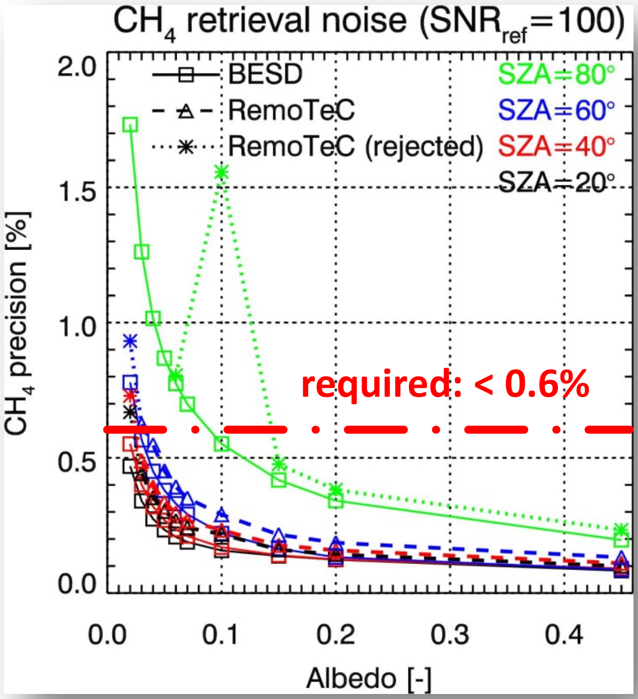


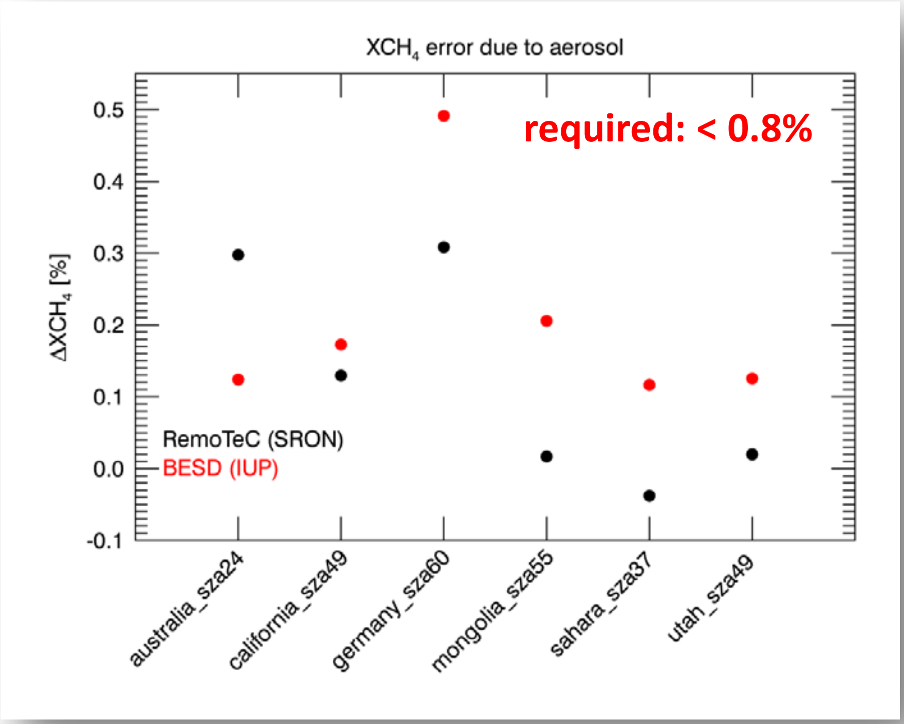
Results for GOSAT



CH4 Verification – BESD (IUP-UB)

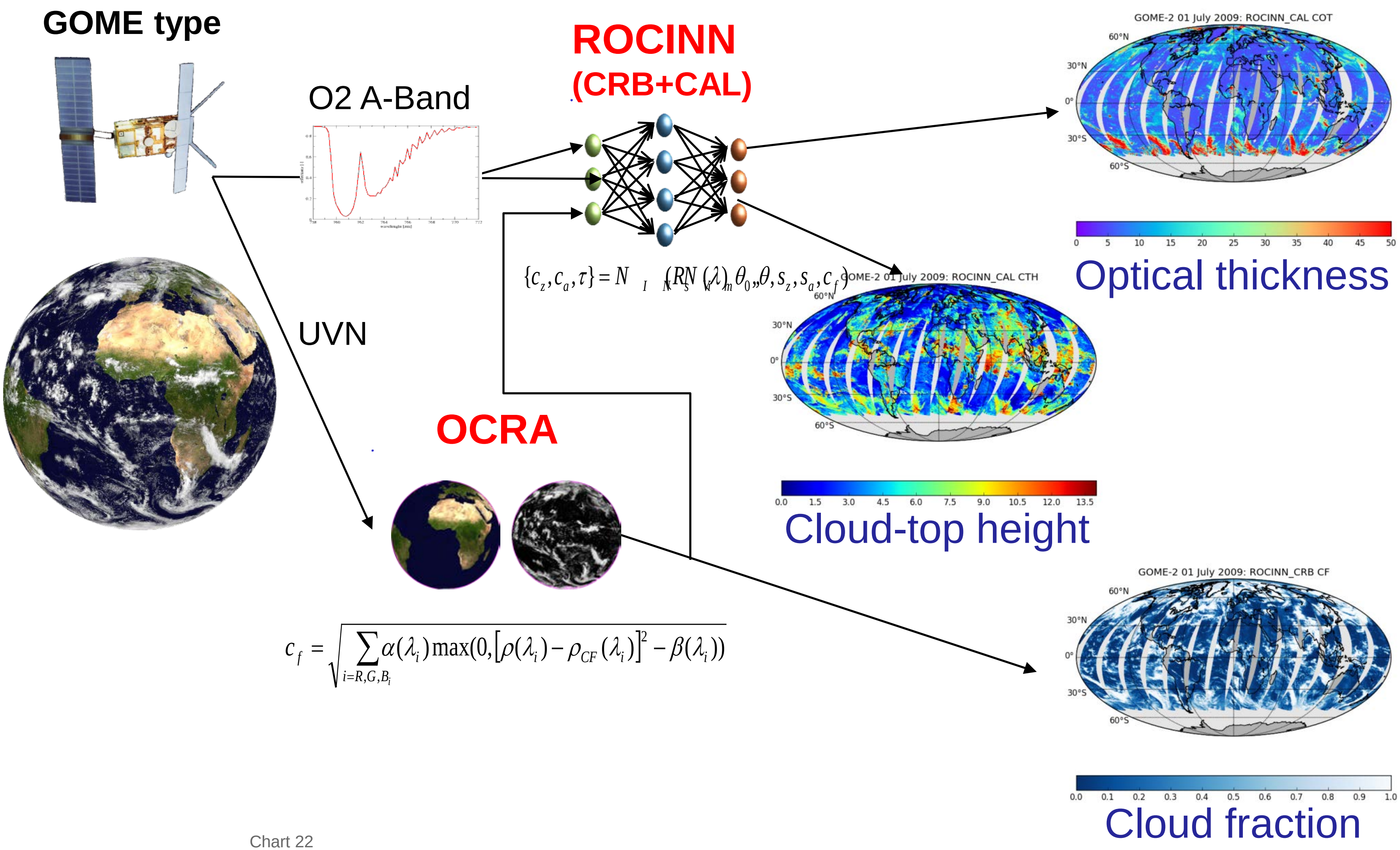
- Same algorithm as for CO verification





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

Clouds Algorithm – OCRA & ROCINN (DLR)



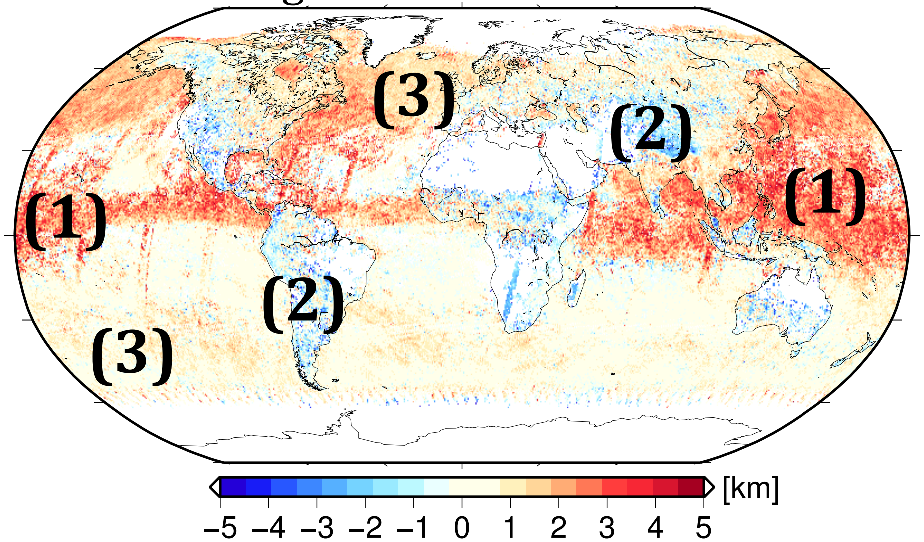
$$\{c_z,c_a,\tau\} = N_I(R_N(\lambda_m),\theta_0,\theta,s_z,s_a,c_f)$$

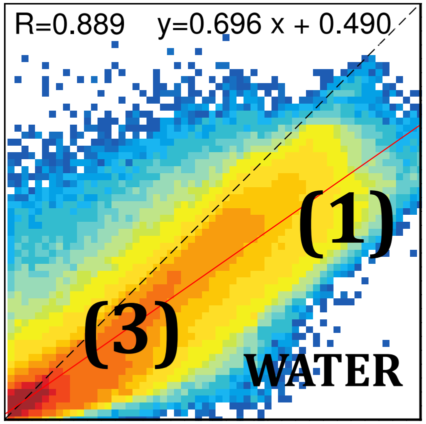
$$c_f = \sqrt{\sum_{i=R,G,B_i} \alpha(\lambda_i)\max(0,[\rho(\lambda_i)-\rho_{CF}(\lambda_i)]^2-\beta(\lambda_i))}$$

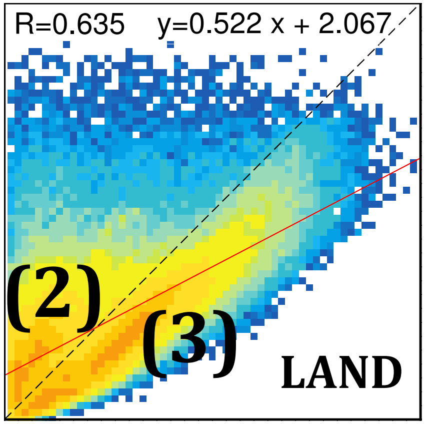
Clouds Verification (IUP-UB, KNMI)

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

Aerosols Index Algorithm (KNMI)

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

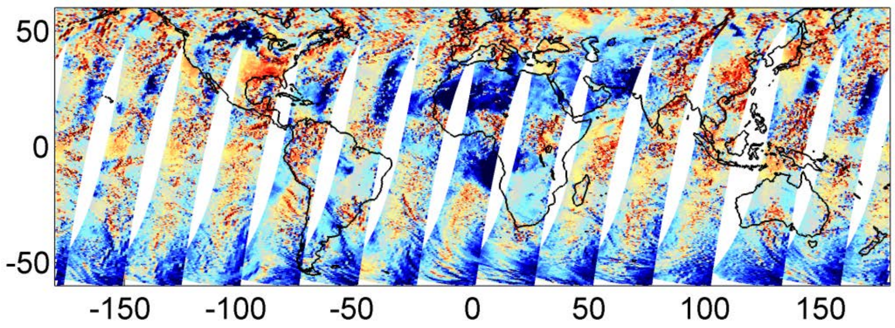
- Prototype algorithm strongly based on operational algorithm (KNMI)
- Wavelength pairs: 340/380 and 354/388 nm
- Auxiliary input:
  - Ozone total column from ECMWF 3h-forecast (for NRT UVAI)
  - Mean surface altitude from digital elevation map (GMTED2010, USGS)
- LUT calculation as for operational algorithm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

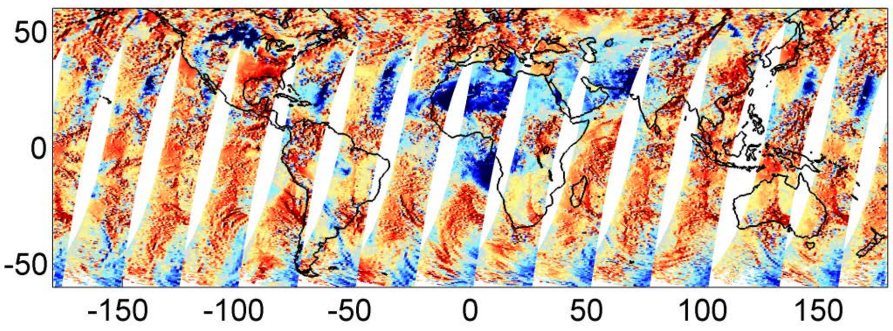
Aerosols Index Verification (MPIC)

- 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)

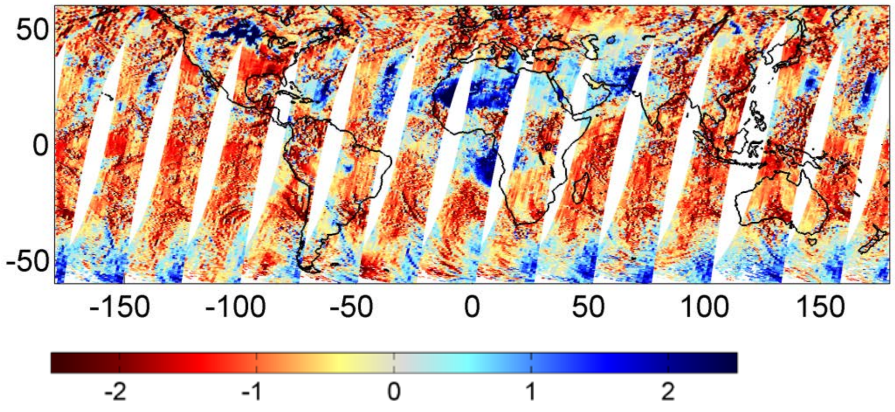
prototype



operational



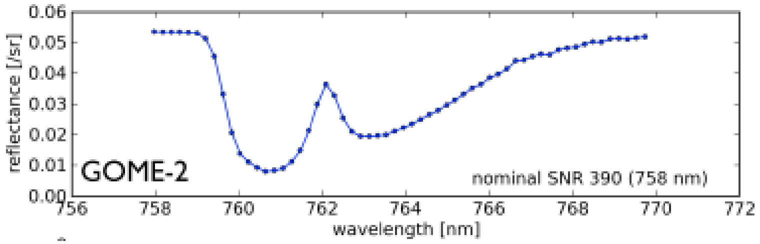
verification



- Qualitative agreement good; more detailed comparison in progress
  - Offset
  - Viewing angle-dependent diff.

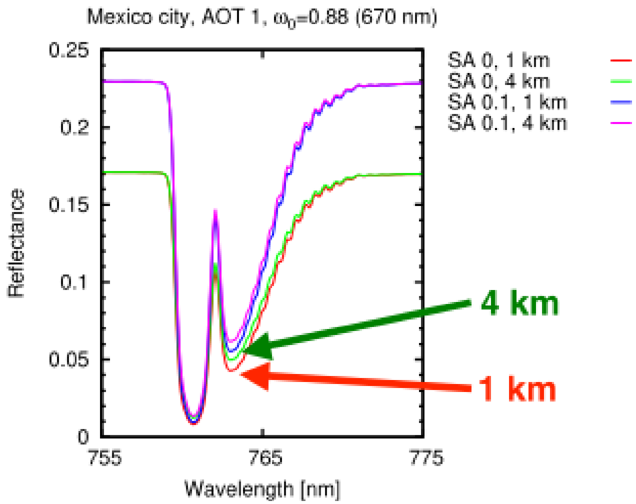
Aerosols Layer Height Algorithm (KNMI)

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

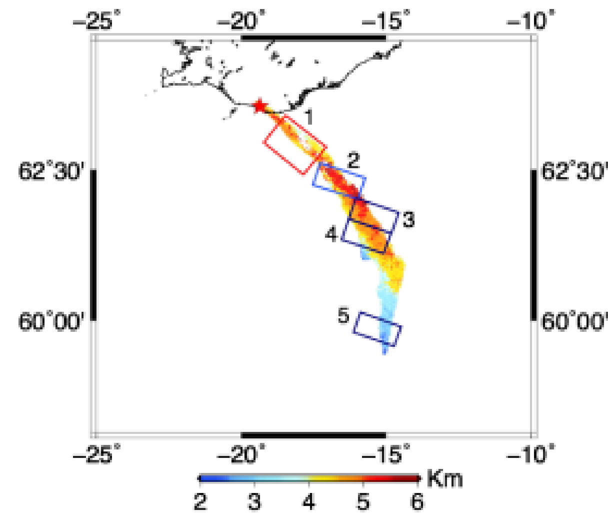


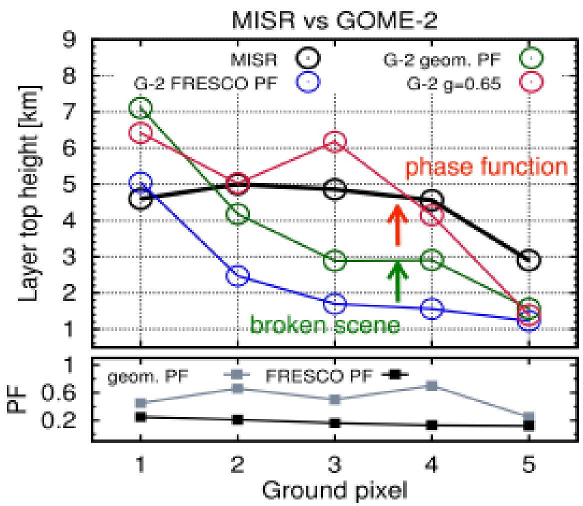
Verification

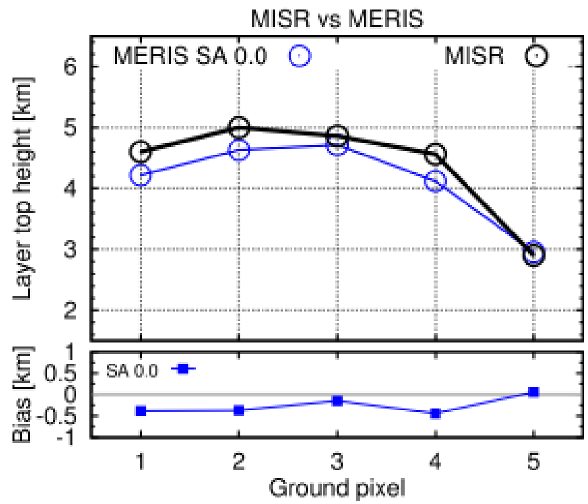
- Optimal estimation algorithm (SCIATRAN)
- Profile parameterization: scattering layer starting at surface
- 2-parameter retrieval: AOT and aerosol layer top height
- Aerosol models from AERONET climatology
- Retrieval using on LUT-based weighting functions

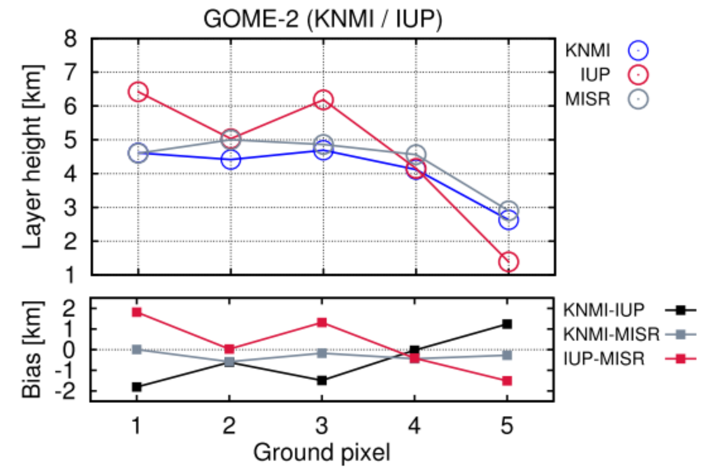
Aerosols Layer Height Verification (IUP-UB)

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





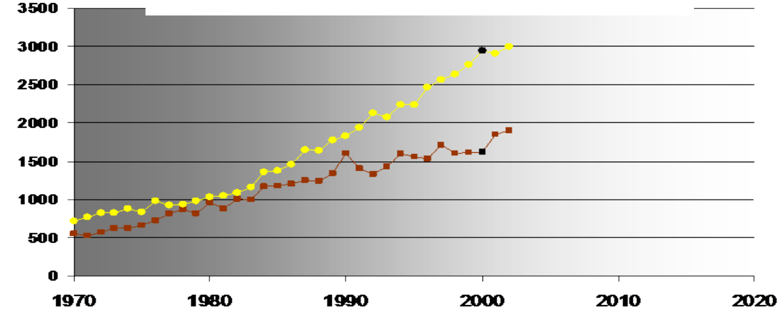




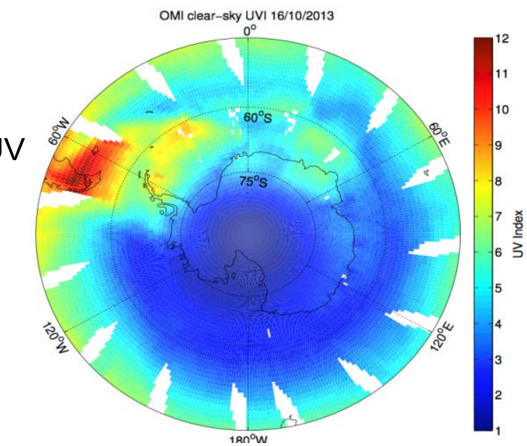
UV* Algorithm (FMI)

- 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**

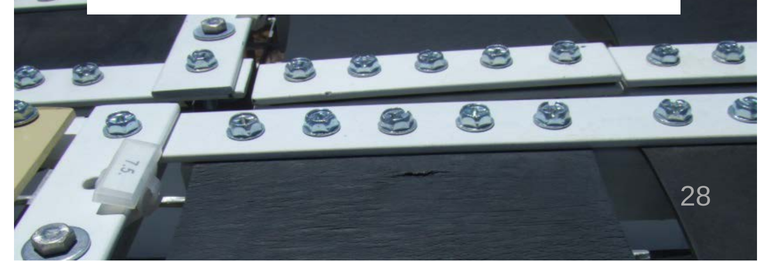
NUMBER OF SKIN CANCERS



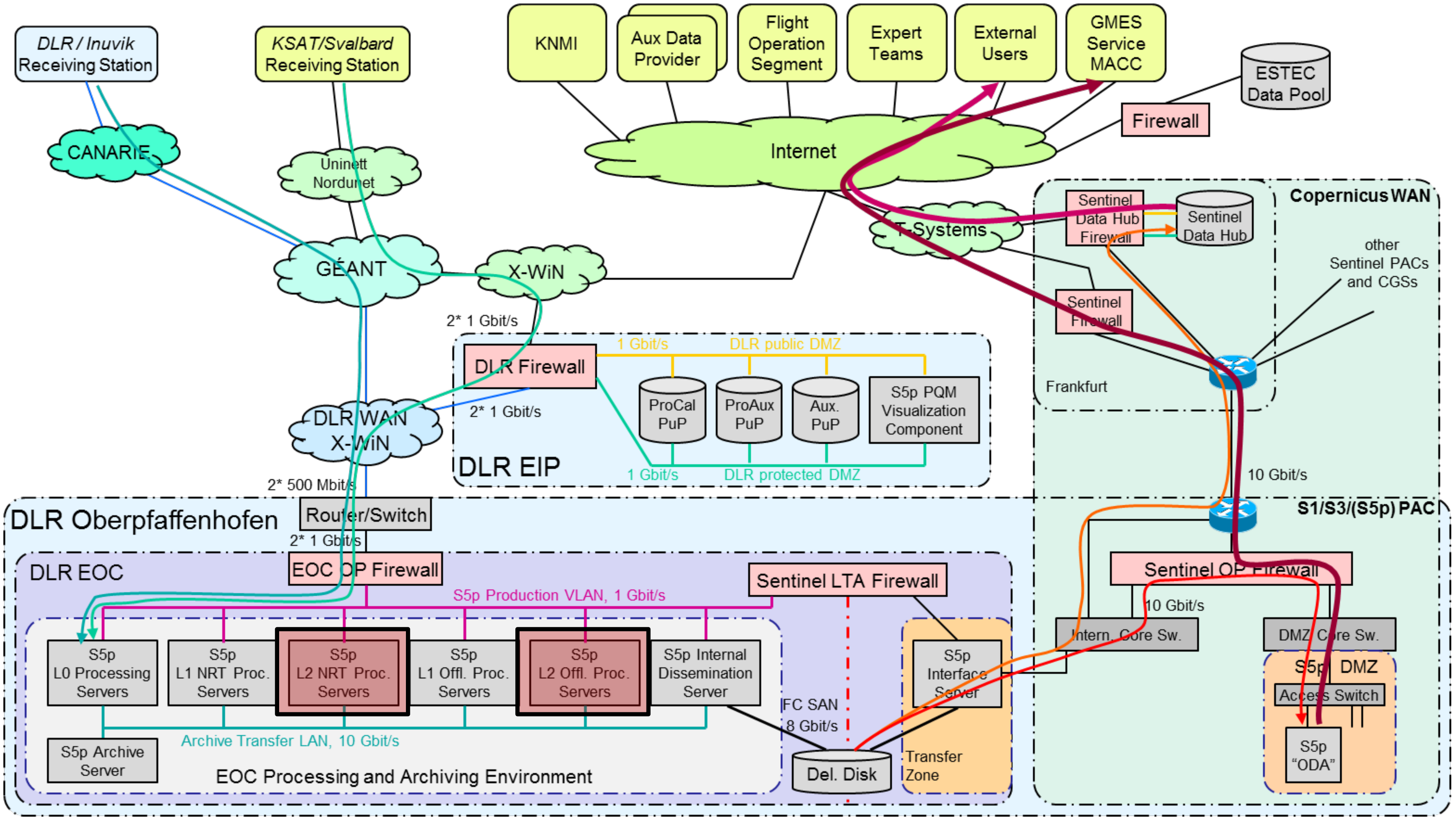
ELEVATED UV
IN OCT 2013



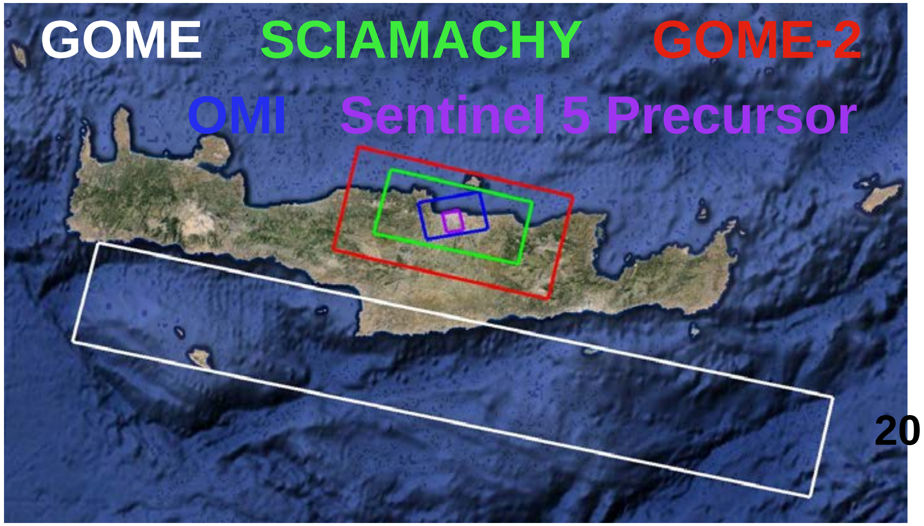
RUBBER UNDER UV EXPOSURE



S5P L2 Processors – PDGS Context

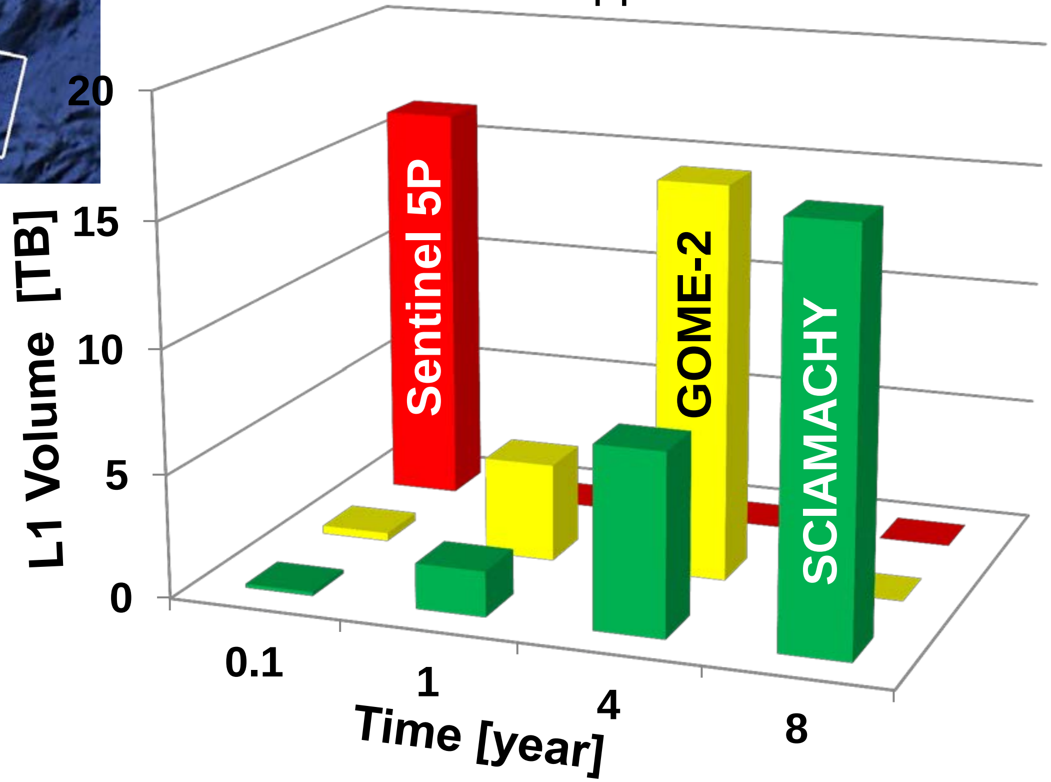


S5P L2 Processors – Big Data Challange



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

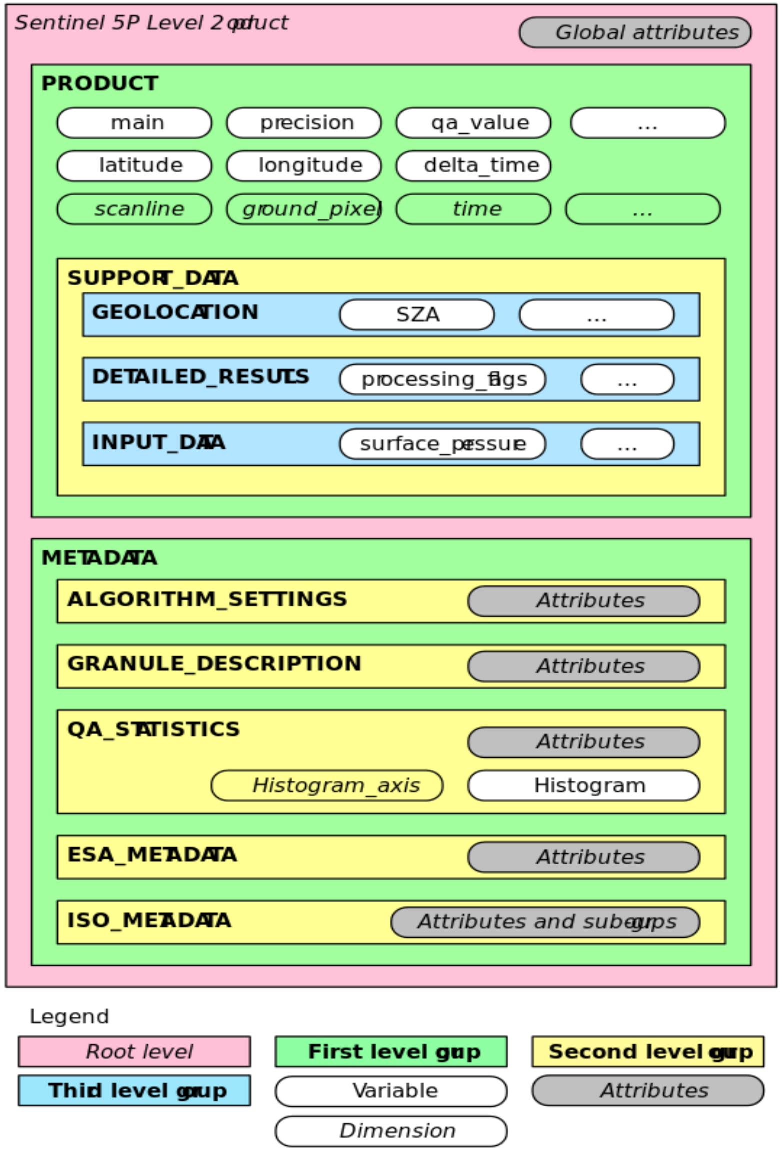


Compared to GOME & OMI:
increase in spectral range
- L1B ~ 35 GB/orbit

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)