Sentinel-4 Geophysical Products for Air Quality and Climate Monitoring

Diego Loyola, German Aerospace Center (DLR)
S4-Teams from ESA L2OP and EUMETSAT AC-SAF

ESA ATMOS Conference
Virtual, 22nd November 2022

DLR

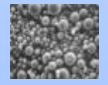
Sentinel-4 Geophysical (Level-2) Operational Products

- S4 L2 Copernicus Products
  - Development phase: ESA project with DLR as prime
  - Operational phase: EUMETSAT

- S4 L2 EUMETSAT AC-SAF Products
  - Development phase: DLR
  - Operational phase: DLR

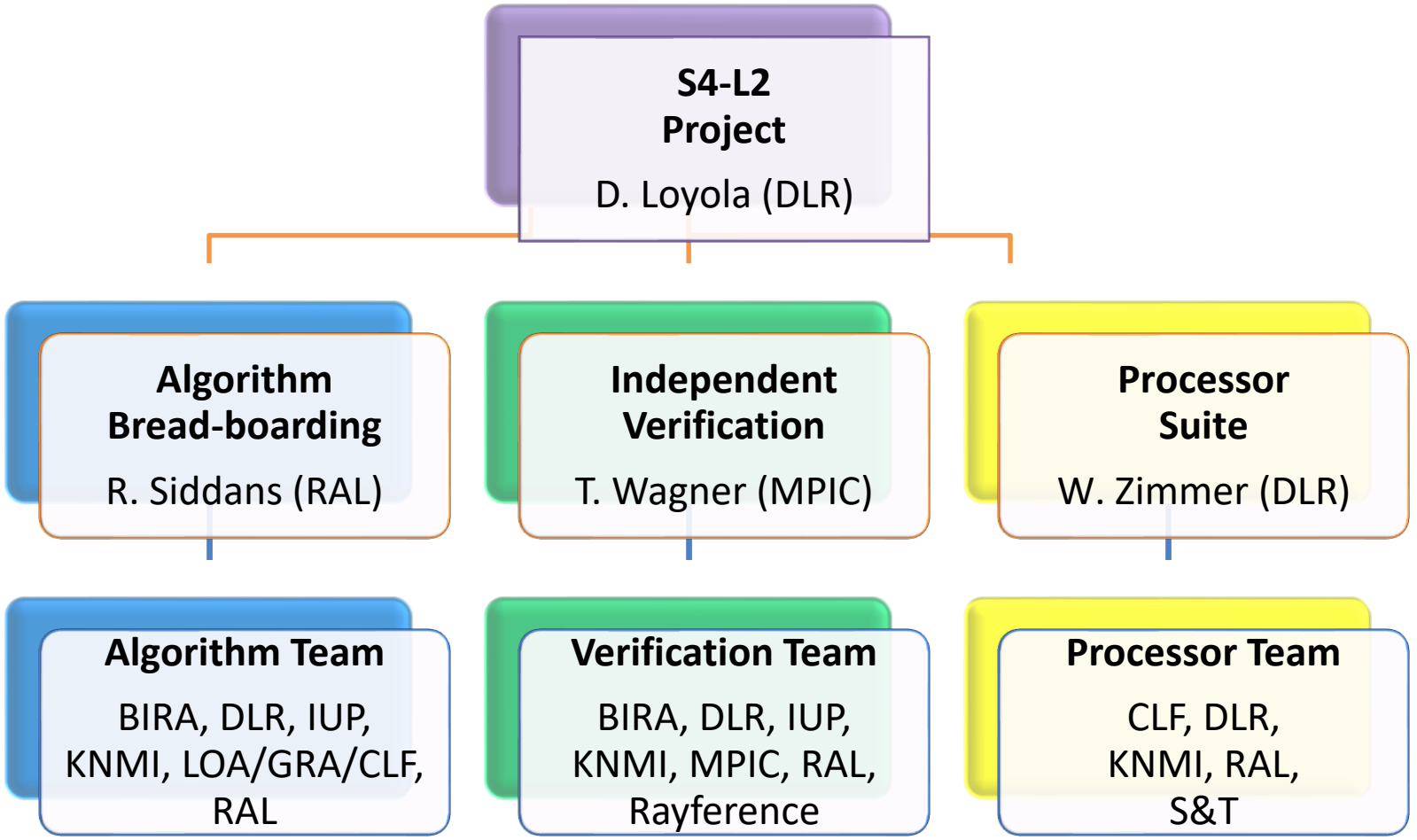
DLR

Sentinel-4 – Geophysical (Level-2) Copernicus Products

		COPERNICUS Applications			
Species	**Parameter**	**Air quality**	**Climate**	**Surface level UV radiation**	**Others**
O_3 	Total column	×			
	Tropospheric column				
NO_2 	Total column	×			
	Tropospheric column				
SO_2 	Total column	×			Volcanic eruptions
HCHO 	Total column	×			
CHOCHO 	Total column	×			
Cloud 	Cloud fraction		×	×	Used as input for other S4 products retrieved from S4 and regridded from FCI
	Optical depth				
	Cloud height				
Aerosol 	Index	×			Used as input for other S4 products Volcanic eruptions
	Optical depth				
	Layer Height				
Surface reflectance	BRDF and white sky albedo			×	Used as input for other S4 products

DLR

Sentinel-4 L2OP ESA/Copernicus Project

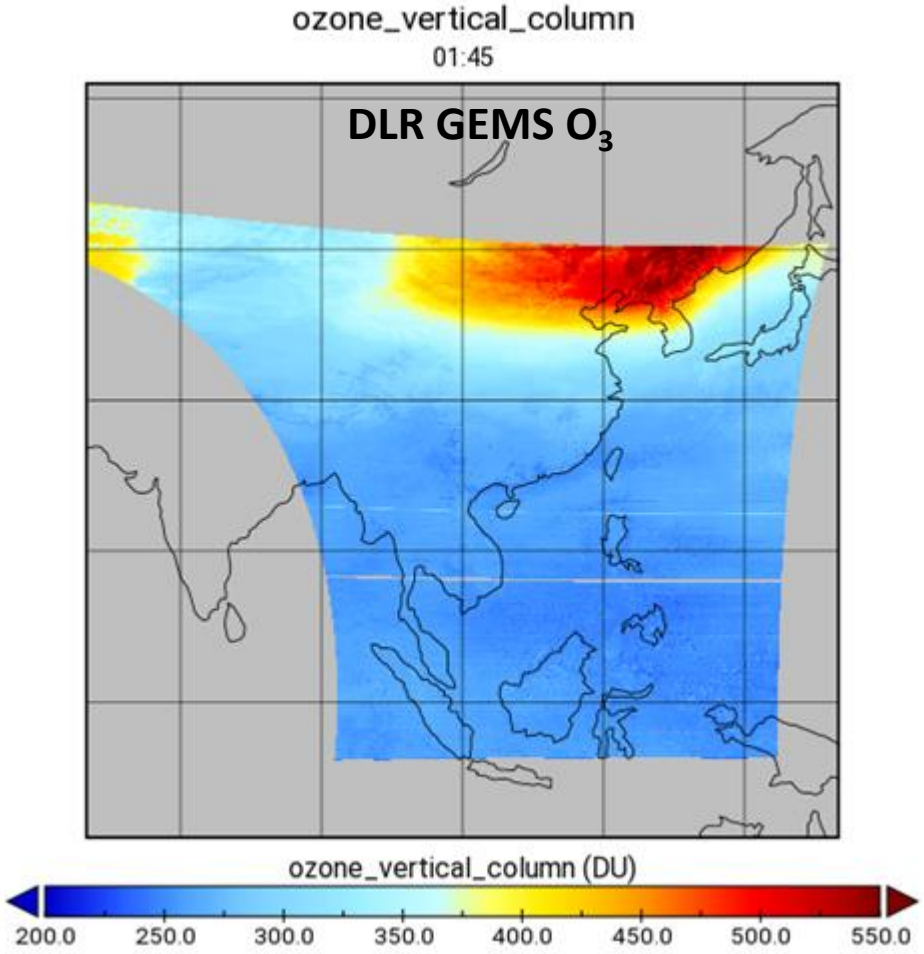


DLR

Sentinel-4 Copernicus – Total Ozone (O_3)

- **Heritage**
  - GOME/SCIA/GOME-2: DOAS with iterative AMF/VCD (Van Roozendael et al., JGR 2006; Loyola et al., JGR 2011; Hao et al., AMT 2014)
  - TROPOMI:
    - OCRA/ROCINN Cloud as Layer (CAL) Loyola et al., AMT 2018
      - No need of ghost-column and intra-cloud corrections
    - Retrieval of surface properties GE_LER Loyola et al., AMT 2020

- S4 algorithm
  - AMF computed using S4 BRDF and the S4 OCRA/ROCINN CAL



Courtesy K-P. Heue (DLR)

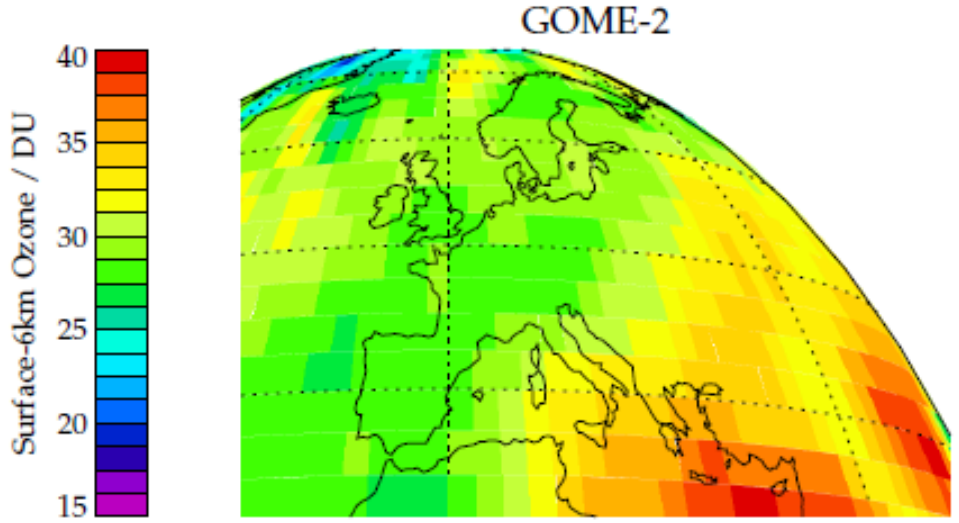
Sentinel-4 Copernicus – Tropospheric Ozone (O_3)

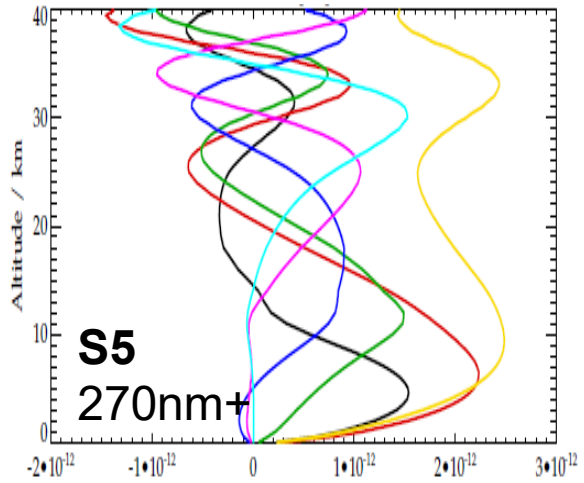
RAL Space

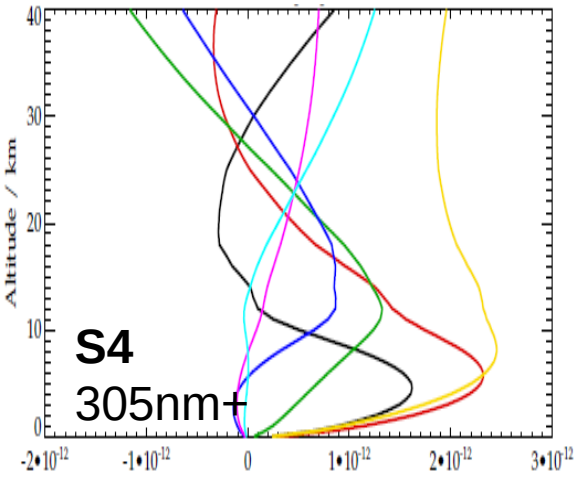
- **Heritage**: ozone profile algorithm developed for GOME
  - Specific emphasis on tropospheric ozone by exploiting the temperature dependence of the Huggins bands

- ESA CCI-ozone selected this scheme to provide full record from GOME-1, SCIAMACHY, GOME-2 and OMI

- S4 has no measurements of Hartley band below 305nm, which provides stratospheric profile information in all previous missions





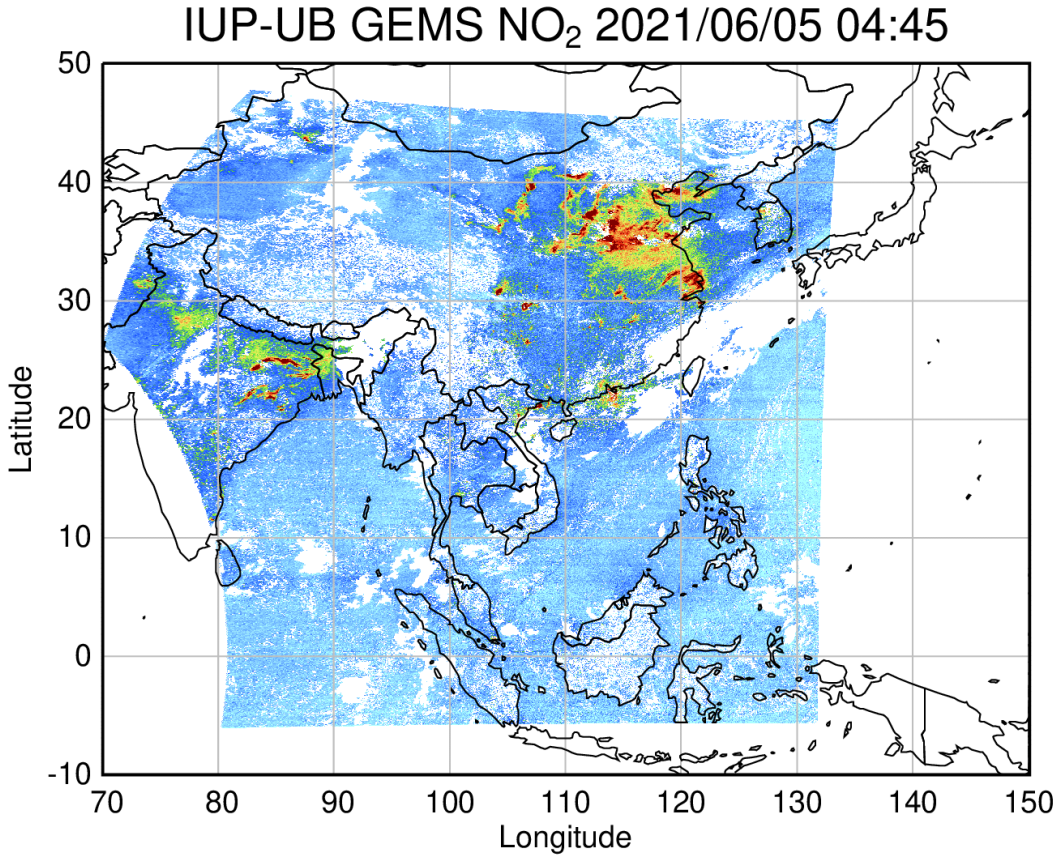


DLR

Sentinel-4 Copernicus – Tropospheric Nitrogen Dioxide NO_2)

- **Heritage**: Standard DOAS retrieval from GOME, SCIAMACHY, GOME-2 , OMI and TROPOMI
  - Stratospheric correction to determine tropospheric slant columns
  - Application of AMFs to determine tropospheric vertical columns

- S_4 algorithm
  - Stratospheric fields from CAMS based on assimilation of S_5(P) and S_4 data
  - BRF effects included in AMFs based on S_4 BRF product
  - A priori NO_2 profiles from high-resolution regional CAMS forecast

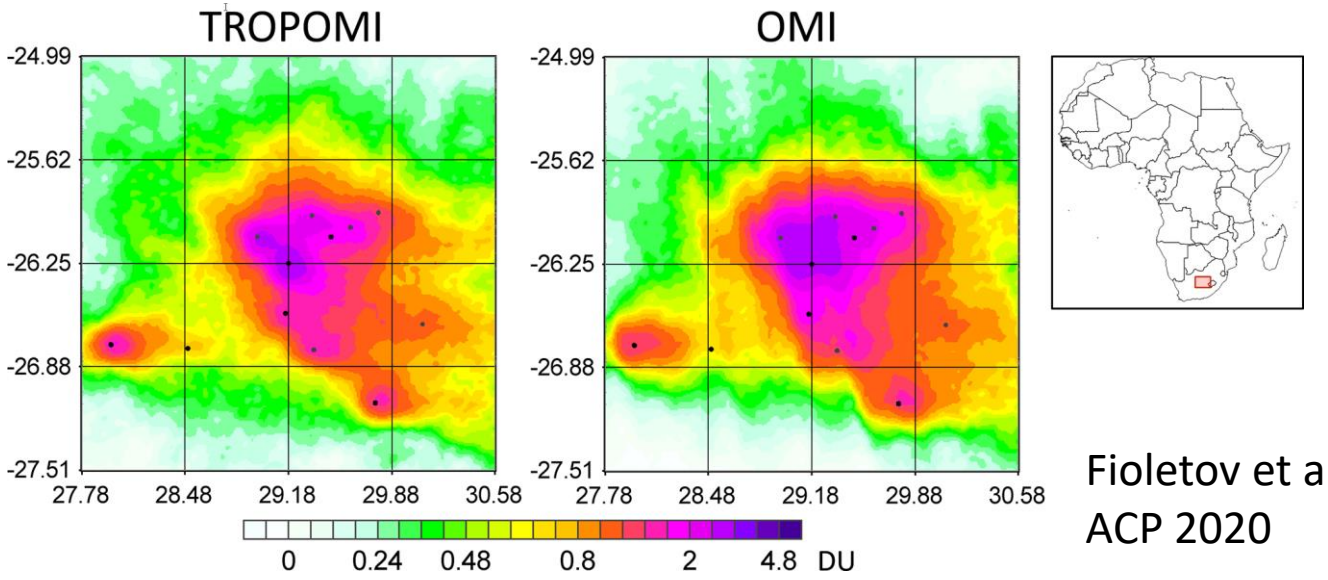


Courtesy A. Richter (IUP-B)

Sentinel-4 Copernicus – Sulfur Dioxide (SO_2)

– **Heritage**: DOAS with one baseline fitting windows plus two alternative windows for high SO_2, similar to the operational algorithm for S5P

– S_4 algorithm
  – Background offset correction
    Screening of volcanic plumes and heavy pollution
  – Conversion to VCD by means of an AMF dependent on other S_4 L2 products: BRF, clouds and aerosol index

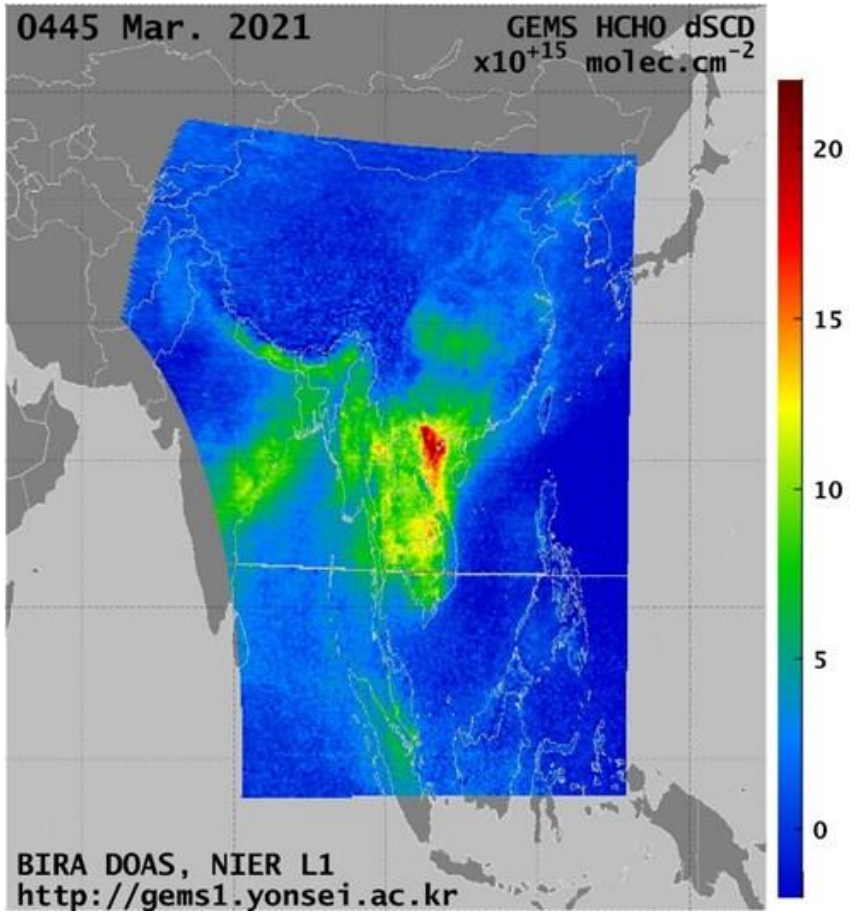


Fioletov et al.,
ACP 2020

Sentinel-4 Copernicus – Formaldehyde (HCHO)

- **Heritage:** Two-window DOAS ([BrO] and [HCHO]), similar to the algorithm for S5P

- S4 algorithm
  - Background offset correction
  - Conversion to VCD by means of an AMF dependent on other S4 L2 products: BRF, clouds and aerosol index
  - Ocean region does not suffice for background correction



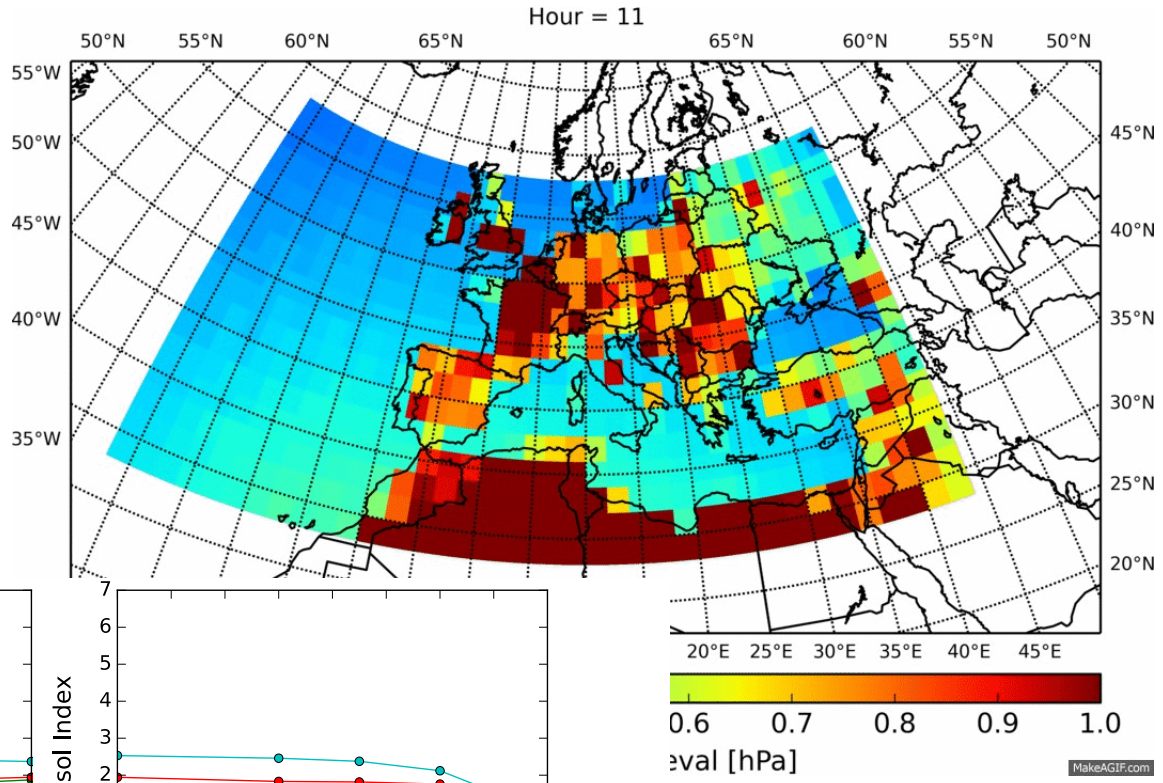
ATMOS P3.5.1, van Gent et al.

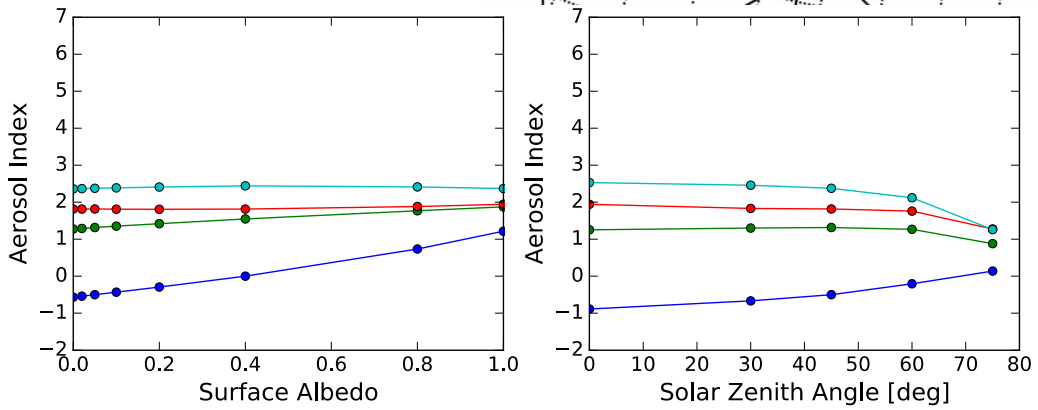
Sentinel-4 Copernicus – Aerosol Layer Height (ALH) and Aerosol Index (AI)

– **Heritage:**
  – ALH algorithm from S5P using information from the O2 A-Band

  – AI algorithm from TOMS using two different pairs

ALH Diurnal Variability of the Retrieval Error



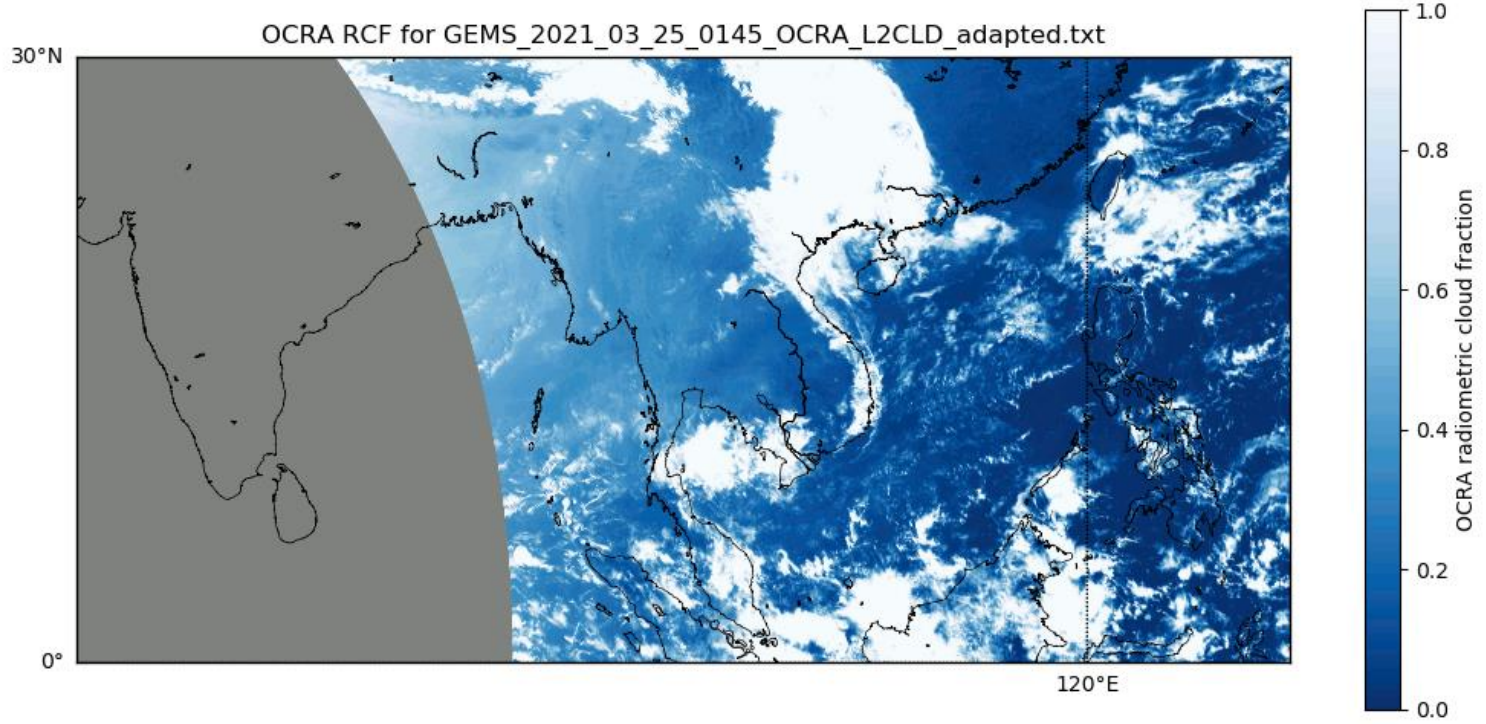


Sentinel-4 Copernicus – Clouds

- **Heritage:** OCRA/ROCINN algorithms used operationally for GOME, GOME-2, and S5P

- OCRA (UV)
  - Cloud fraction

- ROCINN (NIR)
  - CAL
    - Cloud optical thicknes
    - Cloud top height
  - CRB
    - Cloud albedo
    - Cloud height

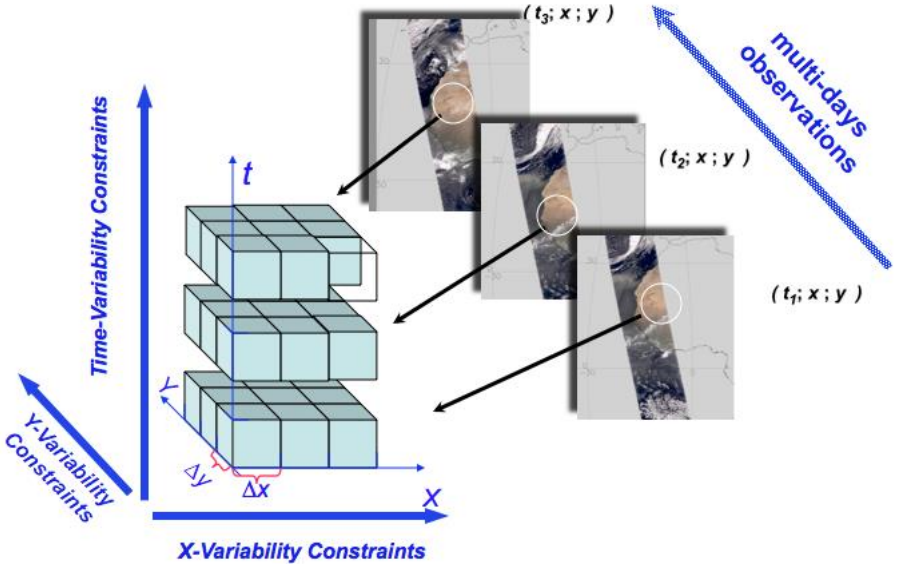


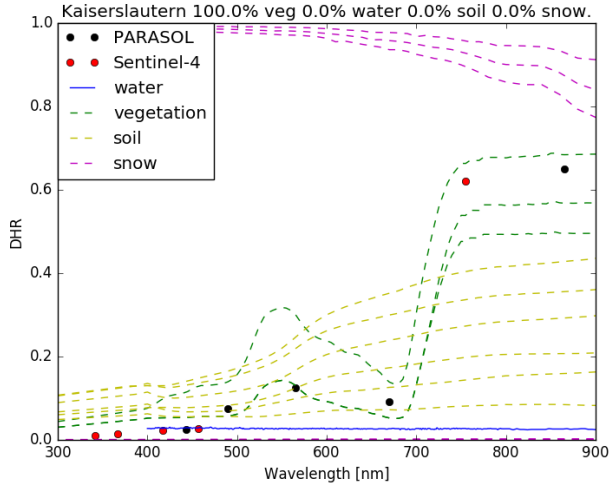
ATMOS 5.1.1, Lutz et al.

Sentinel-4 Copernicus – Surface and AOD

- **Heritage**: GRASP
  - Multi-day retrieval approach, each day with multi-hours measurements
    - More stable and accurate surface reflection retrieval

- S4 algorithm
  - Retrieved products for cloud free conditions:
    - Surface **BRDF** (BRF, DHR, White Sky Albedo)
    - **AOD**
  - Daily Gapless Surface Reflectance
    - Surface **BRDF** for different wavelengths 342, 367, 410, 443, 490, 755 nm

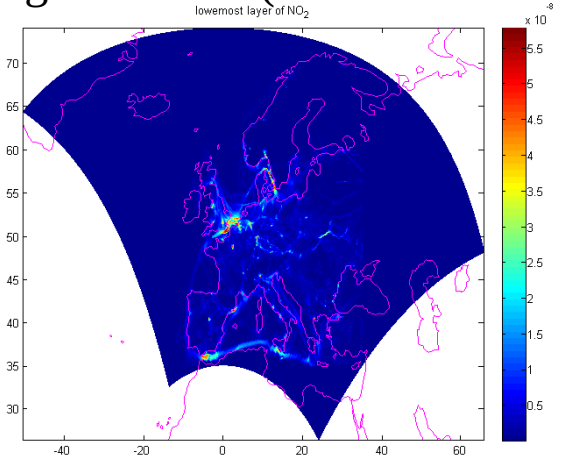




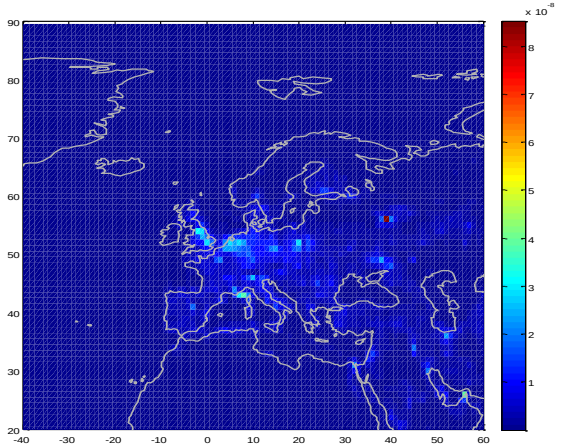
Sentinel-4 Copernicus – Geophysical Reference Data

MAX-PLANCK-INSTITUT FÜR CHEMIE

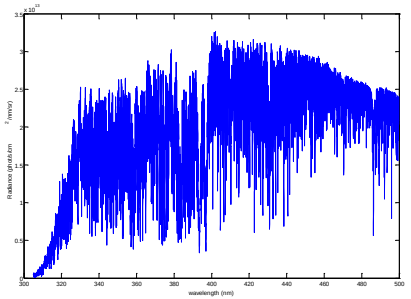
High resolved (LOTOS EUROS)

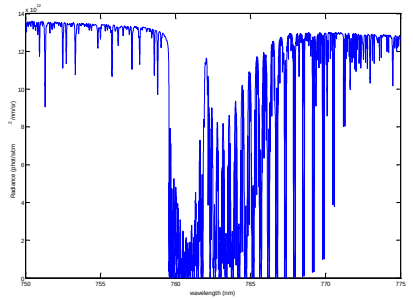


TM5 1x1 everywhere else

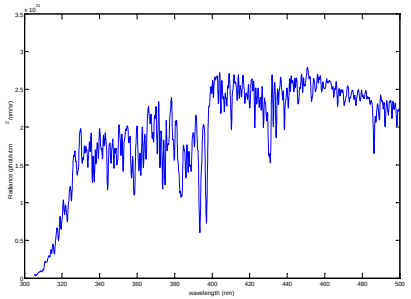


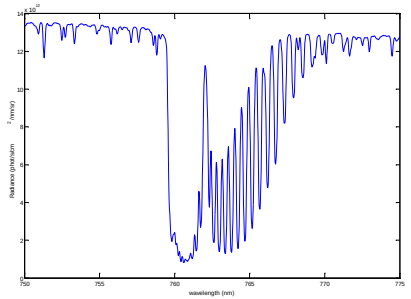
RTM





S4 Instrument





Sentinel-4 Copernicus – Geophysical Reference Data (2)

- 2*5 days (summer + winter) with 3x3 pixel boxes
- fully cloudy, partially cloudy, aerosol and SO_2 scenarios
- 17 locations across FOV
- Clouds with
  - CTH= 2, 4, 8 km
  - COT= 5, 20
  - CF= varying

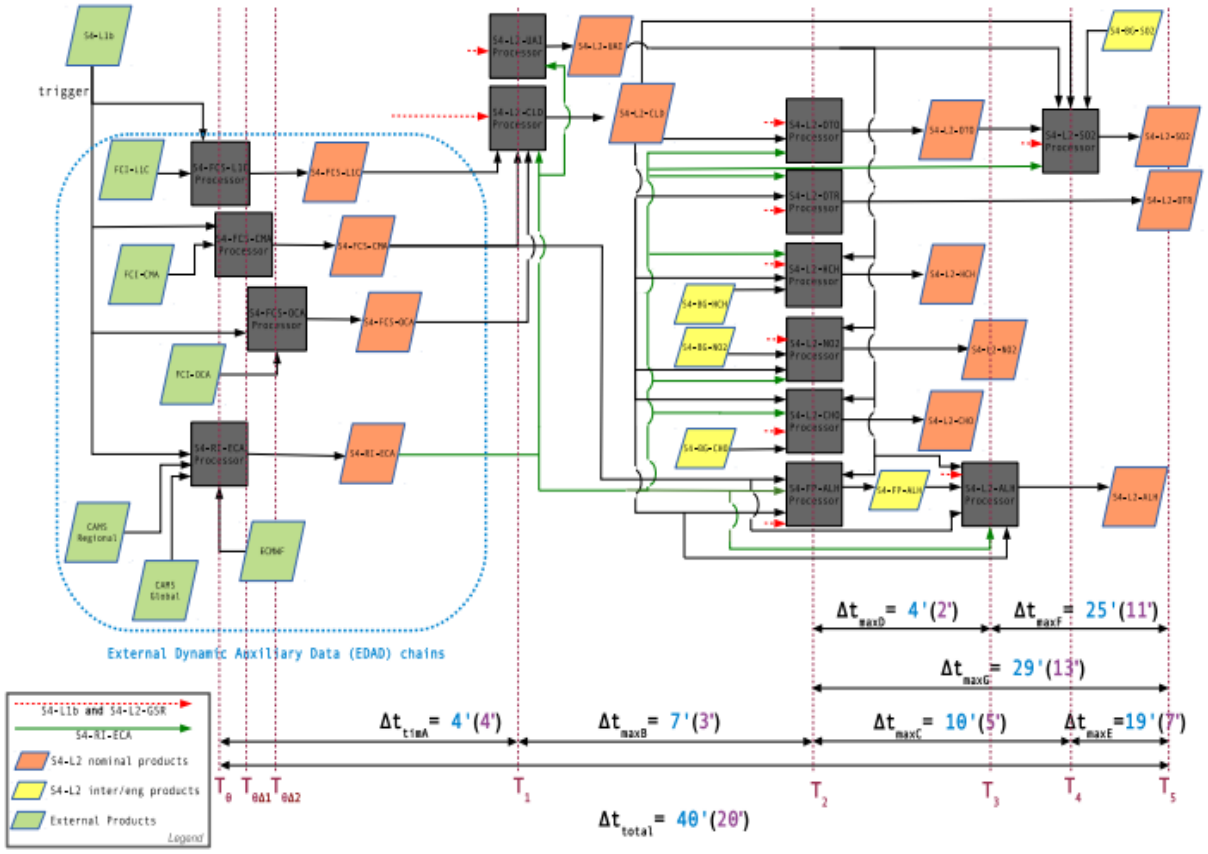
Sentinel-4 L2 Operational Processors (L2OP)

- The L2OP suite comprises 18 processors
  - Complex interdependencies and processing time constraints

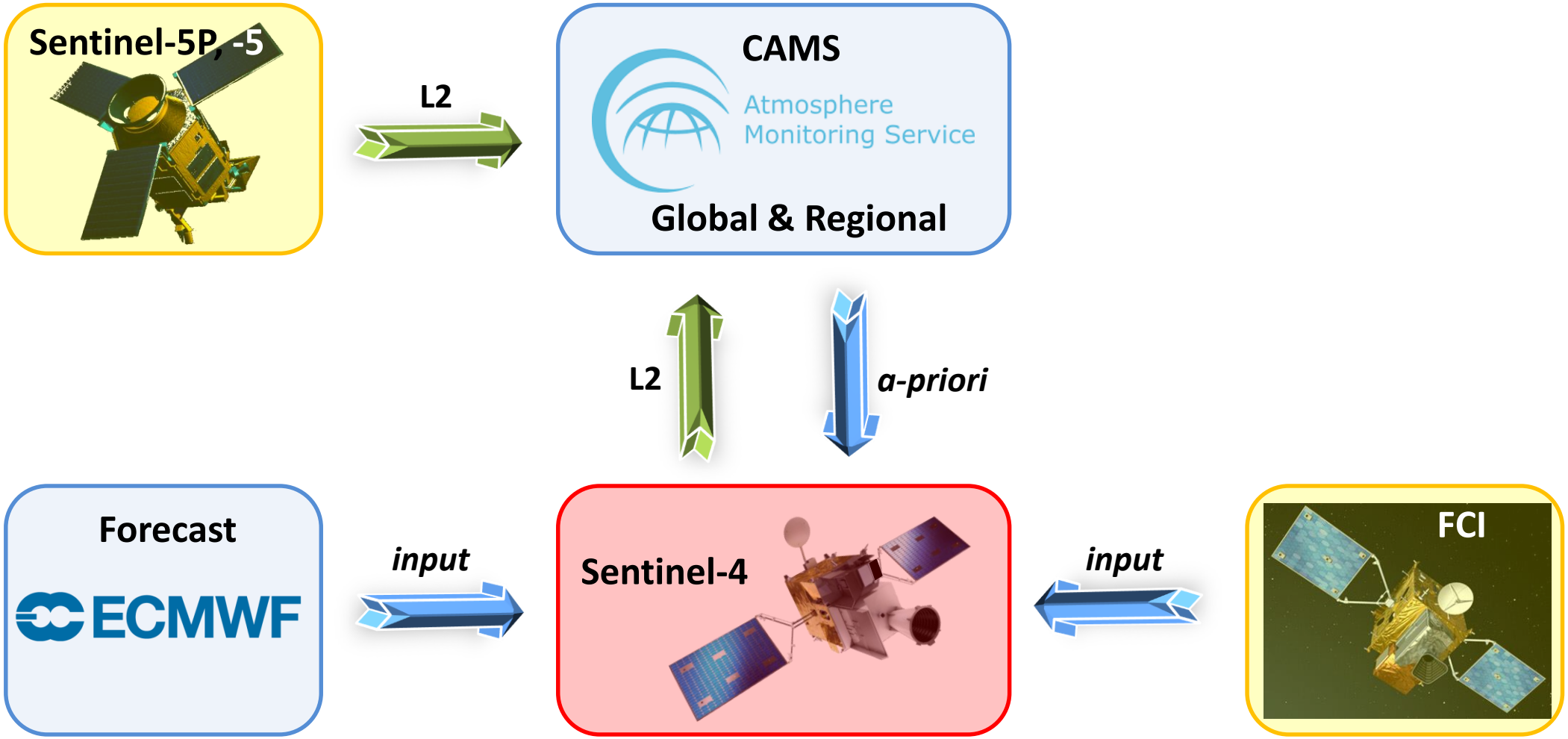
- L2OP mock-up successfully integrated into the EUMETSAT L2PF ground-segment

- L2OP version 1 under development
  - 12 processors already delivered
  - 6 processors planned for early 2022

- L2OP version 2 to be ready before launch
  - Including the latest algorithm improvements
  - Possible updates due to S4 on-ground calibration



Sentinel-4 L2OP Interactions with ECMWF, CAMS, FCI, and Sentinel-5P/-5



DLR

Sentinel-4 Geophysical (Level-2) Operational Products

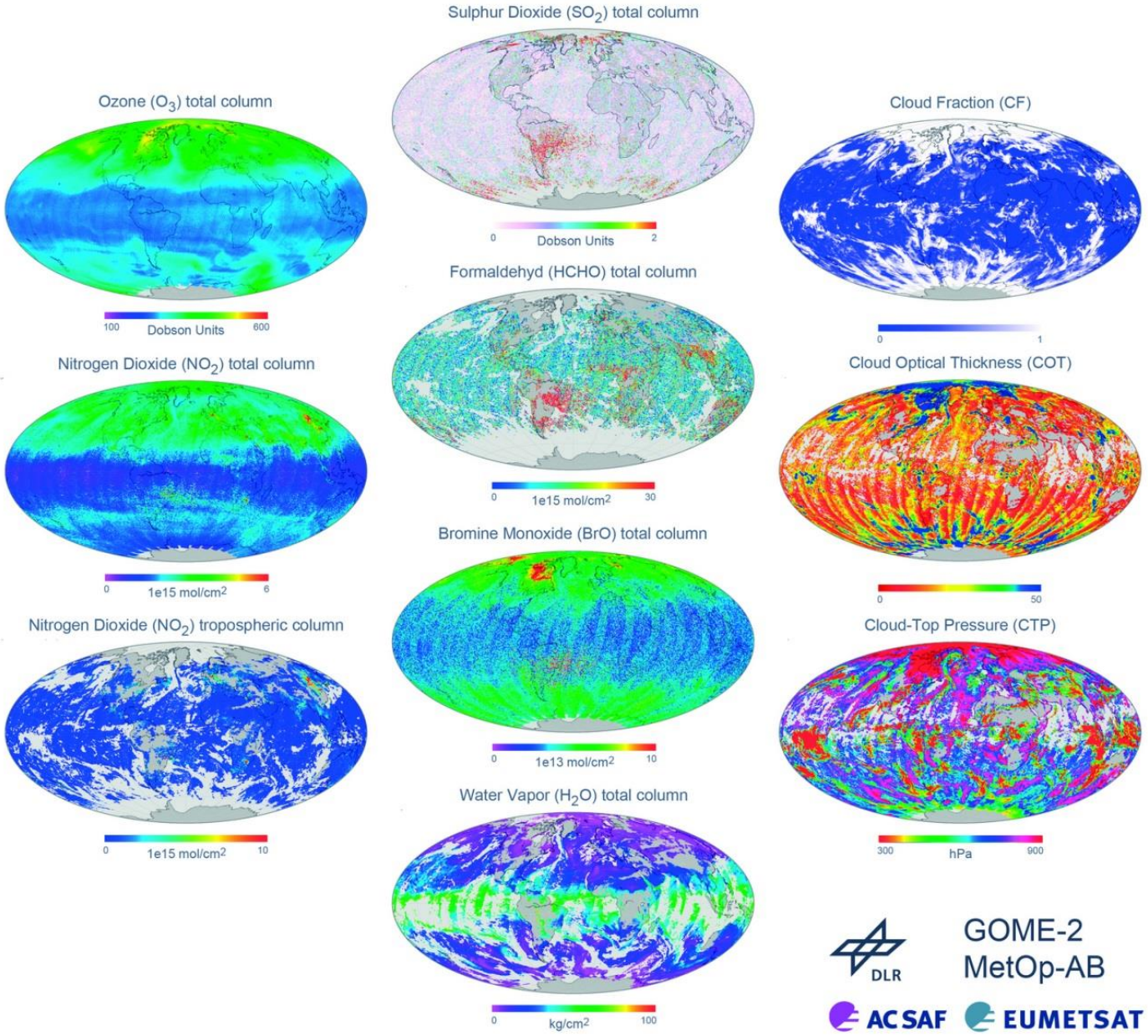
- S4 L2 Copernicus Products
  - Development phase: ESA project with DLR as prime
  - Operational phase: EUMETSAT

- S4 L2 EUMETSAT AC-SAF Products
  - Development phase: DLR
  - Operational phase: DLR

DLR

EUMETSAT AC-SAF

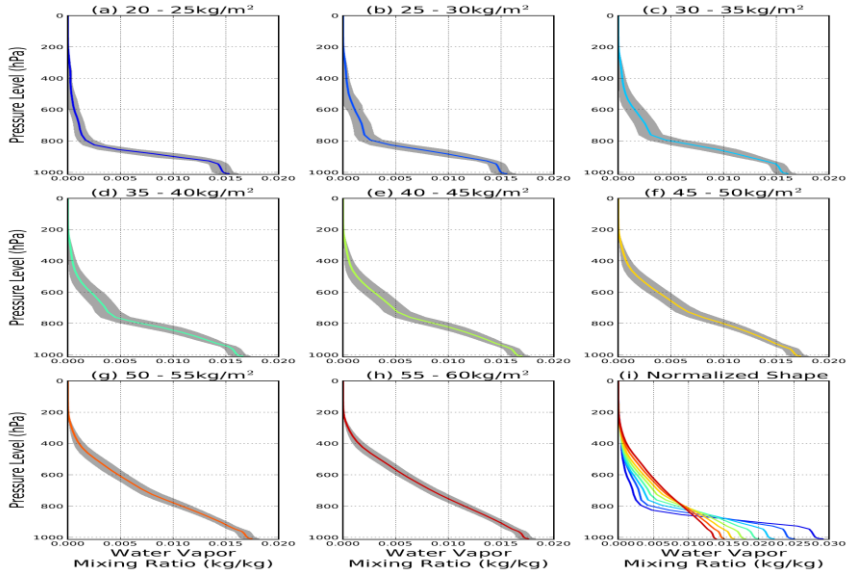
- MetOp series extended the GOME/ERS-2 and SCIAMACHY data record
  - 26 years of UVN ozone, water vapour and other trace gases
- DLR provides a large number of operational GOME-2 products from MetOp-A, MetOp-B, and MetOp-C
- AC-SAF products generated by DLR are used by Copernicus CAMS
- DLR will provide AC-SAF Sentinel-4 and Sentinel-5 products
  - **Total Column Water Vapor (TCWV)**
  - **SO2 Layer Height**
  - …

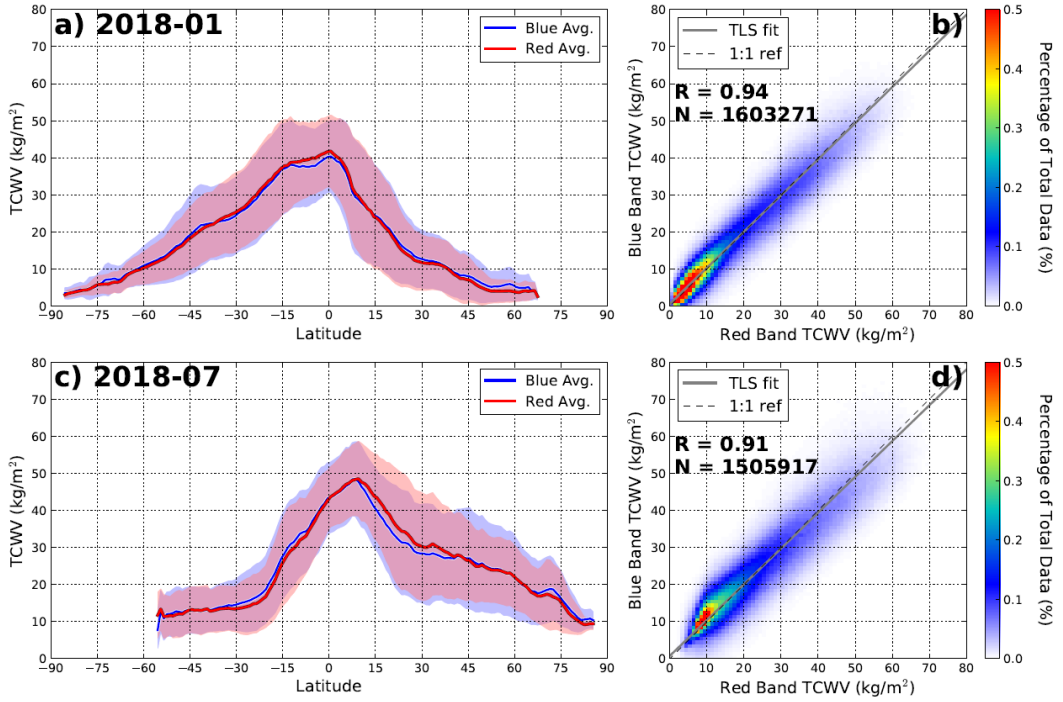


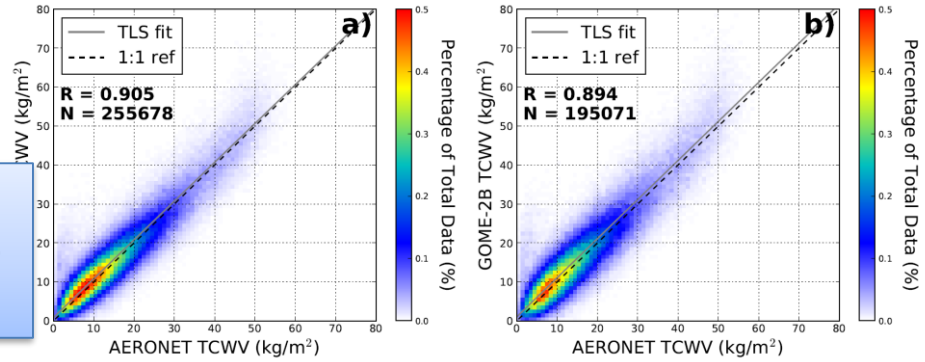
DLR

TCWV Blue Band – GOME-2/MetOp

- DOAS fitting in the blue band
- Iterative AMF/VCD calculation
  - WV profile climatology classified as function of TCWV based on 11 years of ERA-Interim



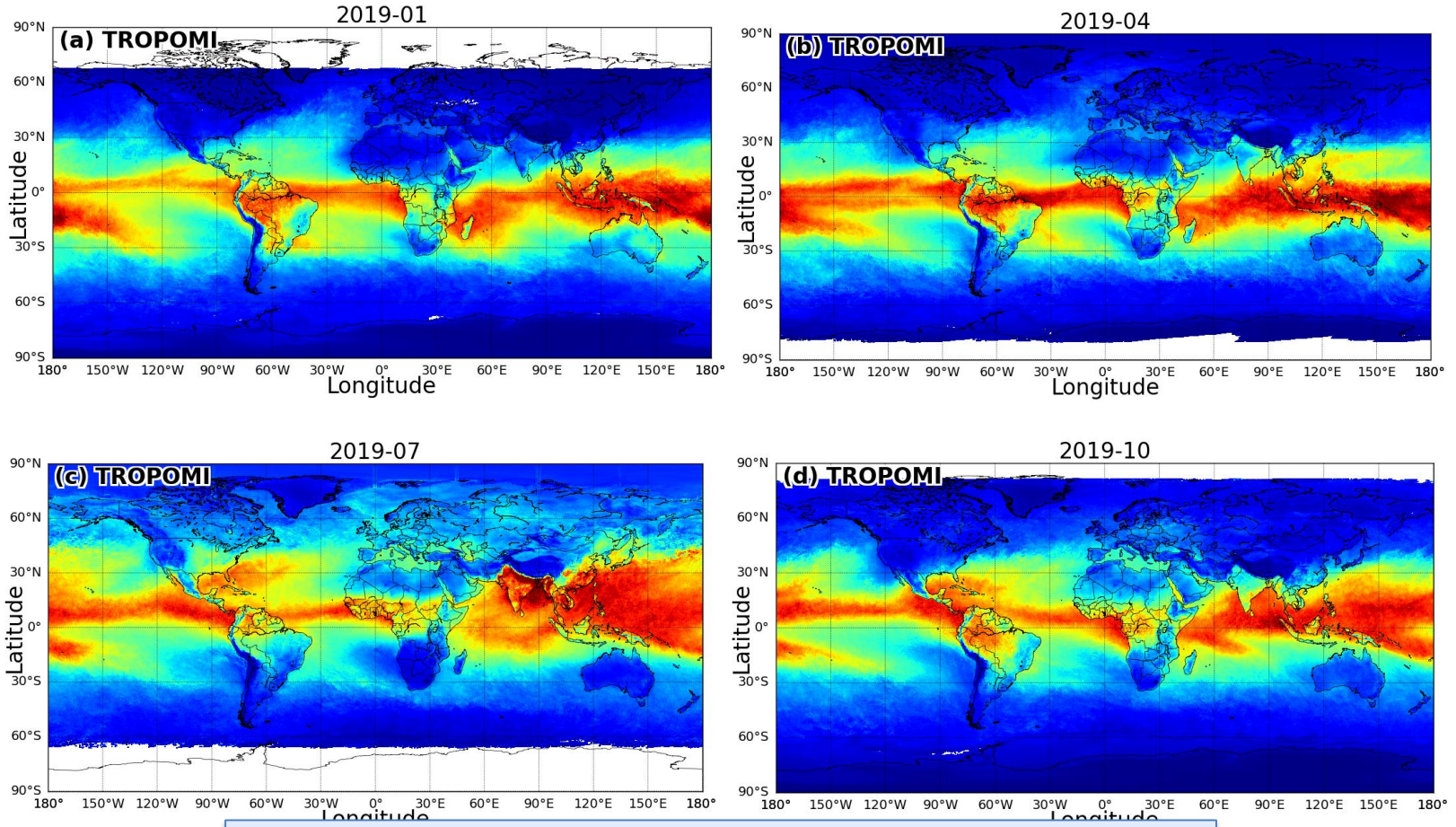


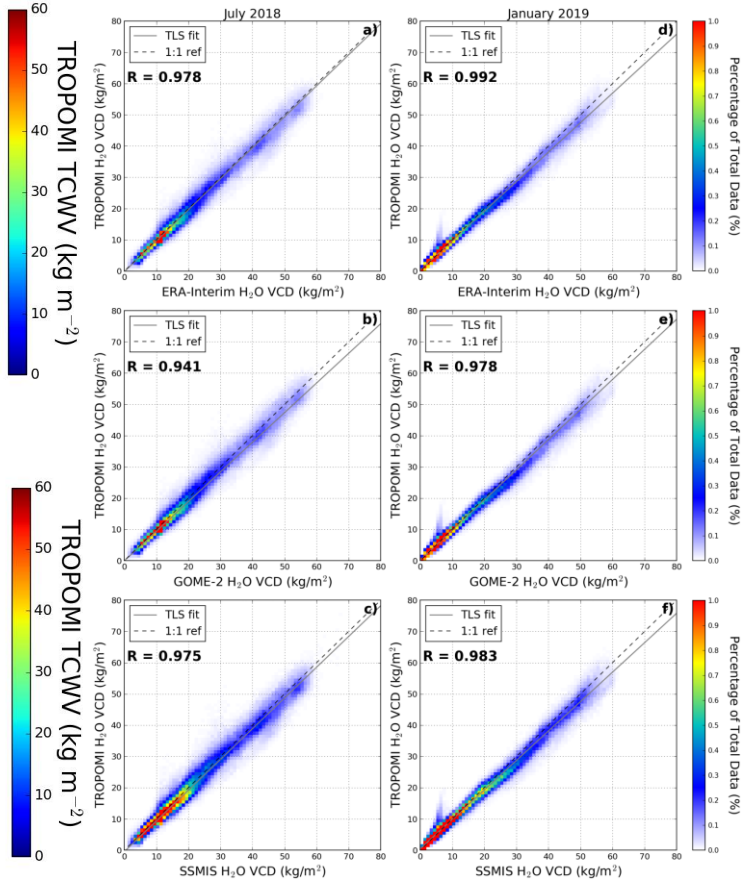


Chan K. L., Valks P., Slijkhuis S., Köhler C., Loyola D., Retrieval of total column water vapor from GOME-2 visible blue spectra, AMT 2020

DLR

TCWV Blue Band – TROPOMI/Sentinel-5P PAL





Chan K. L., Xu J, Slijkhuis S., Valks P., Loyola D.,
TROPOMI observations of total column water vapour:
algorithm and validation, submitted 2021

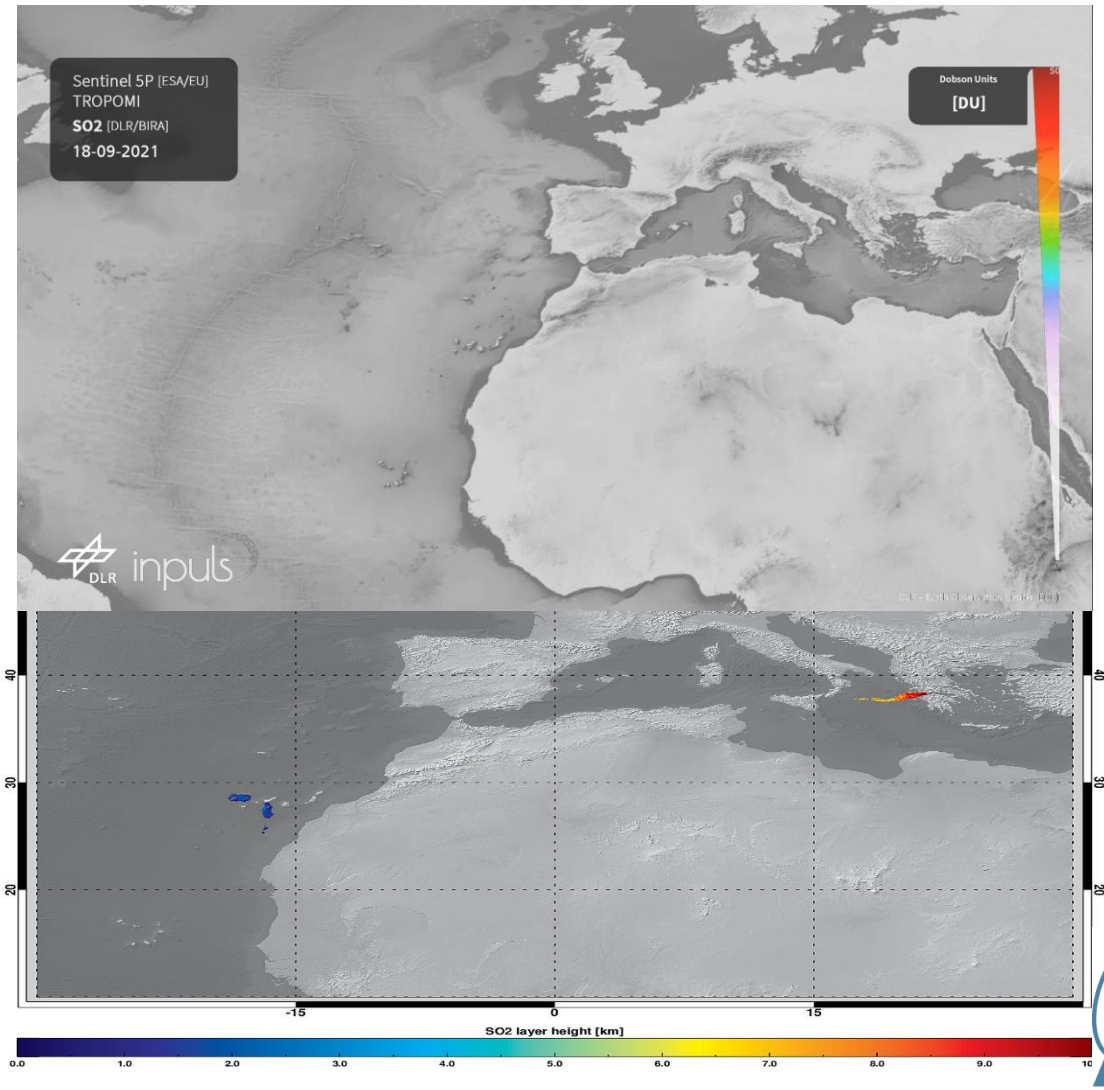
ATMOS 3.1.3, Chan et al.

SO2 Layer Height

- FP_ILM (Full-Physics Inverse Learning Machine)
  - PCA + Neural Network retrieval
  - Extremely fast and accurate SO2 LH
  - Processing speed: ~3ms / pixel
  - Accuracy: <2km (SO2 VCD > 20 DU)

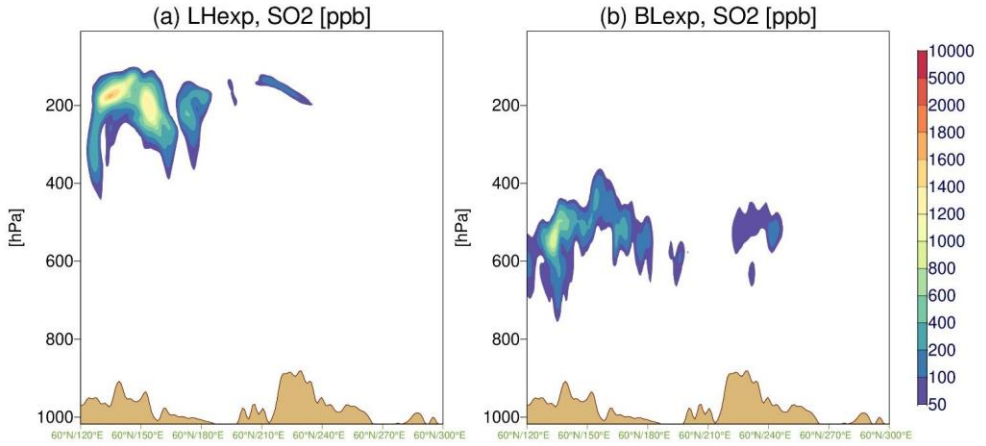
- Applied to:
  - GOME-2/MetOp
    - Efremenko et al. 2017
  - TROPOMI/S5p
    - Hedelt et al. 2019
  - OMI/AURA
    - Fedkin et al. 2020

Cumbre Vieja & Etna 2021



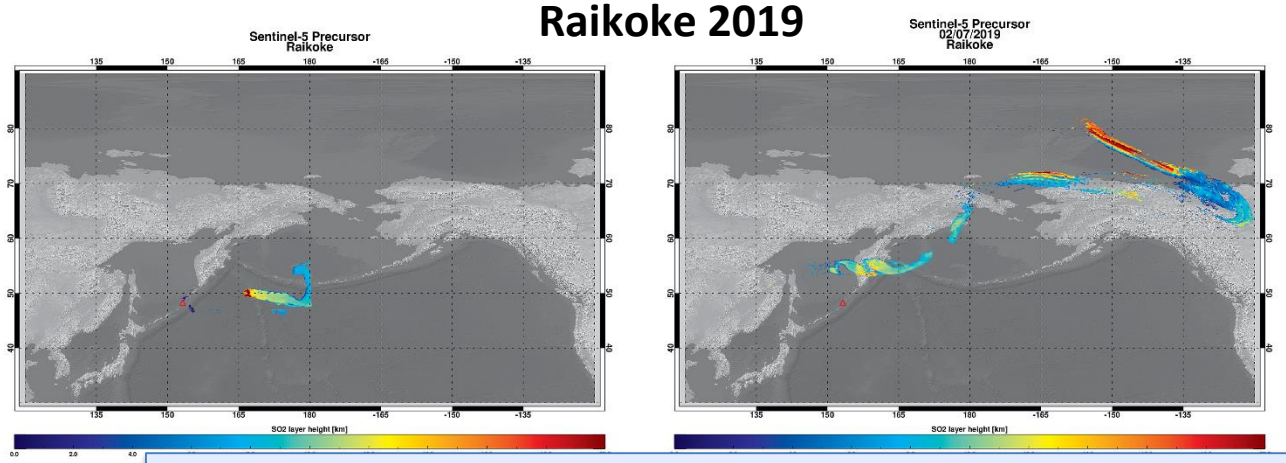
SO2 Layer Height – TROPOMI/Sentinel-5P

– Retrieval further optimized in ESA S5P+I: SO2LH, data being assimilated in CAMS



A. Inness, M. Ades, D. Balis, D. Efremenko, J. Flemming, P. Hedelt, ME. Koukouli, D. Loyola, R. Ribas, The CAMS volcanic forecasting system utilizing near-real time data assimilation of S5P/TROPOMI SO2 retrievals, GMD 2021

Raikoke 2019



ME. Koukouli, K. Michailidis, P. Hedelt, IA. Taylor, A. Inness, L. Clarisse, D. Balis, D. Efremenko, D. Loyola, RG. Grainger, C. Retscher, Volcanic SO_2 Layer Height by TROPOMI/Sentinel-5P: validation against IASI/MetOp and CALIOP/CALIPSO observations, submitted 2021

– Semi-operational NRT S5P SO2 LH provided by DLR INPULS

– Immediate tweet @DlrSO2: https://twitter.com/DlrSo2

ATMOS 5.3.1, Hedelt et al.

BIRA: Michel Van Roozendael, Jeroen van Gent, Christophe Lerot, Isabelle De Smedt, Nicolas Theys, Huan Yu

CLF: Michael Aspetsberger, Octavian Cuibus, Andrei Filip, Verena Lanzinger, Florian Steinschorn

DLR: Diego Loyola, Ana del Aguila Perez, Çağrı Erciyes, Klaus-Peter Heue, Ronny Lutz, Victor Molina Garcia, Fabian Romahn, Birgit Wunschheim, Walter Zimmer

ESA: Norrie Wright, Olivier Le Rille, Ben Veihelmann

GRASP: Pavel Lytvynov, Anton Lopatin

IUP-B: Andreas Richter, Lisa Behrens

KNMI: Pepijn Veefkind, Martin De Graaf, Maarten Sneep

LOA: Oleg Dubovik

MPIC: Thomas Wagner, Steffen Beirle, Janis Pukite

S&T: Daniele Fantin, Andrei Kukharenka

RAL: Richard Siddans, , Andy Smith

RAY: Yves Govaerts, Marta Luffarelli

EUMETSAT AC SAF ATMOSPHERIC COMPOSITION MONITORING

DLR: Pieter Valks, Ka-Lok Chan, Pascal Hedelt, Klaus-Peter Heue, Stefan Kiemle, Sander Slijkhuis, Walter Zimmer