ATMOS 2021 Conference Report and User Recommendations



ATMOS-2021

Conference Report and User Recommendations

1	Introduction
2	List of Acronyms
3	Objectives. Themes. Scientific Committee and Session Chairs
4	Plenary Sessions Summary & Highlights
	/ 1 Science from Space & Current Missions
	4.1 Science nom space & current missions
	4.3 International Satellites Missions and Products
	4.4 Future Missions – Copernicus Sentinels
	4.5 Future Missions – Earth Explorers & Earth Watch
	4.6 Future Missions – Earth Explorer Candidates
	4.7 The FORUM Mission
	4.8 Aeolus Mission Data Exploitation
	4.9 Air Quality
	4.10 Ozone
	4.11 Greenhouse Gases
	4.12 Aerosols
	4.13 Clouds
	4.14 Water Vapour
	4.15 Volcanic Emissions
	4.16 OCIO, BrO, Glyoxal

J.4 AUUSUIS & JUIIALE
5.5 Clouds and Water Vapour
5.6 FORUM & Infrared Observations
5.7 Volcanic Emissions
5.8 Other Trace Gases and Atmospheric Processes
5.9 Calibration & Validation

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1. Introduction

In the context of the EO Science for Society Programme Element, the European Space Agency (ESA) has organised the **ATMOS-2021 Atmospheric Science Conference** (https://atmos2021.esa.int/) on the topical theme Atmosphere, aimed at exploiting data from ESA and EO Missions for science and application development. The conference took place as a virtual event on 22–26 November 2021. The purpose of this conference was to provide scientists and data users with the opportunity to present first-hand and up-to-date results from their ongoing research and application development activities by using data from past and current atmospheric missions like Copernicus SentineI-5P, Aeolus and ESA Third Party Missions. Another aspect was discussing activities regarding future missions. This document presents the outcome of ATMOS-2021 and aims at suggesting priorities for a roadmap concerning the initiatives in Atmospheric Chemistry and Dynamics and will help to further shape the next generation of R&D activities in the frame of the ESA Earth Observation Programme.

Event statistics











AAI	Aerosol Absorbing Index
AAOD	Absorbed Aerosol Optical Depth
AATSR	Advanced Along-Track Scanning Radiometer
AC	Atmospheric Composition
ACCO	Above Cloud Column Ozone
ACE	Atmospheric Chemistry Experiment
ACE-FTS	Atmospheric Chemistry Experiment Fourier Transform Spectrometer
ACOS	Atmospheric CO2 Observations from Space
ACTRIS	Aerosols, Clouds and Trace gases Research Infrastructure
AERONET	Aerosol Robotic Network
AI	Aerosol Index
AIRS	Atmospheric Infrared Sounder
IRWAVE	Advanced Infra-Red WAter Vapour Estimator
ALADIN	Atmospheric Laser Doppler Instrument
ALARM	multi-hAzard monitoring and earLy wARning system
ALH	Aerosol Layer Height
ALTIUS	Atmospheric Limb Tracker for Investigation of the Upcoming Stratosphere
AMF	Air Mass Factor
ANN	Artificial Neural Network
AOD	Aerosol Optical Depth
AODC	Coarse Aerosol Optical Depth
AODF	Fine Aerosol Optical Depth
APEX	Airborne Prism Experiment
QA	Air Quality

	Atmospharic Padiation Maasuromont usar facility US
	Autospheric Radiation Measurement user facility, 05 Above see level
	Ground-based component of the IATAC campaign
	Atmospheric I TDAR
ΔΙΙΤΗ	Aristotle University of Thessaloniki, Greece
Δνς	Automated Validation Server
BAOUNTN	Roundary-laver Δir Quality-analysis Using Network of Instruments
BASCOE	Belgian Assimilation System for Chemical ObsErvations
BTRA-TASB	The Royal Belgian Institute for Space Aeronomy, Belgium
BBR	Broad-Band Radiometer
BRDF	Bidirectional Reflectance Distribution Function
BrO	Bromine monoxide
BrONO2	Bromine nitrate
C3S	Copernicus Climate Change Service
CAIRT	Changing Atmosphere InfraRed Tomography Explorer
CALIOP	Cloud-Aerosol LIDAR with Orthogonal Polarisation
CALIPSO	Cloud-Aerosol Lidar and Infrared Pathfinder Satellite Observation
CAL/VAL	Calibration/Validation
CAMS	Copernicus Atmosphere Monitoring Service
CAS	Centre for Advanced Study, The Netherlands
CAS	Chinese Academy of Sciences, China
CCD	Convective Cloud Differential algorithm
CCI	Climate Change Initiative
CCMI	Chemistry-Climate Model Initiative



CDR	Climate Data Records	
CFC	Chloro-Fluoro-Carbon	
CH4	Methane	
СНОСНО	Glyoxal	
CHORA Cloud Height adjusted Ozone Reference Algorithm		
CHOVA Cloud Height induced Ozone Variation Analysis		
CIBR	Continuum Interpolated Band Ratio	
CISAR	Combined Inversion of Surface and Atmosphere pRoperties algorithm	
CLONO2	Chlorine nitrate	
CLOUDNET Data pipeline to process and distribute cloud remote sensing data		
CMAM-39 Canadian Middle Atmosphere Model v39		
CMIP6	Coupled Model Intercomparison Project Phase 6	
CNIT	National Intercollegiate Consortium for Telecommunications, Italy	
CNN	Convolutional Neural Networks	
CNR	National Research Council, Italy	
CNR-IAC	National Research Council-Institute for applied mathematics, Italy	
CNR-IFAC	National Research Council-Institute of Applied Physics, Italy	
CNR-INO	National Research Council- Institute of Optics, Italy	
CNR-ISAC	National Research Council- Institute of Atmospheric Sciences and Climate, Italy	
CNRS	Centre national de la recherche scientifique, France	
CO	Carbon monoxide	
CO2	Carbon dioxide	
CO2M	Carbon Dioxide Monitoring mission	
COBRA	Covariance-Based Retrieval Algorithm	
COCCON	Collaborative Carbon Column Observing Network	
COH NOAA	Cohesive Data	
COMPO-IFS	Composition Integrated Forecast System	

CPR Cloud Profiling Radar

CrIS	Cross-track Infrared Sounder
CRB	Clouds as Reflecting Boundaries model
СТМ	Chemical Transport Model
DARCLOS	Detection AlgoRithm for CLOud Shadows
DAWN	Doppler Aerosol Wind LIDAR
DDS	Diagnostic DataSet
DECSO	Daily Emissions Constrained by Satellite Observations
DISC	Data Innovation and Science Cluster
DIVA	Demonstration of an Integrated approach for the Validation and exploitation
	of Atmospheric missions
DLER	Directional Lambertian Equivalent Reflectivity
DLR	Deutsches Zentrum für Luft- und Raumfahrt, Germany
DNN	Deep Neural Network
DOAS	Differential Optical Absorption Spectroscopy
DSTREAM	Directionally Dependent Stratospheric Estimation Algorithm
DU	Dobson Units
EarthCARE	Earth Clouds and Radiation Explorer
EC	European Commission, Belgium
ECMWF	European Centre for Medium-Range Weather Forecasts, UK
ECSAT	European Centre for Space Applications and Telecommunications, UK
ECV	Essential Climate Variable
EEA	European Environment Agency, Denmark
	European Geosciences Union
EM2//SUN FIIR	Remote Sensing analysers dedicated for atmospheric measurements
	SWISS Federal Laboratories for Materials Science and Technology
ENVISAI	ESA Environmental Satemile Earth's Next-generation TCE mission
ENIILE	Earth Observation
EU	



EPS-SG EUMETSAT	Polar System - Second Generation	GEO	Geosynchronous Equatorial Orbit
ERA ECMWF	Reanalysis dataset	GEOS-Chem	Model of atmospheric chemistry driven by meteorological input
ERP	External Reconstruction Problem		from the Goddard Earth Observing System
ERS-2	European Remote Sensing satellite 2	GHGs	GreenHouse Gases
ESA	European Space Agency, France	GHGSat	Greenhouse gas satellite constellation
ESRIN	European Space Research Institute, Italy	GLORIA	Gimballed Limb Observer for Radiance Imaging of the Atmosphere
ESTEC	European Space Research and Technology Centre, The Netherlands	GIoSSAC	Global Space-based Stratospheric Aerosol Climatology
Eubrewnet	European Brewer Network	GOME-2	The Global Ozone Monitoring Experiment-2
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites, Germany	GOMOS	Global Ozone Monitoring by Occultation of Stars
EVDC	ESA atmospheric Validation Data Centre	GOSAT	Greenhouse gases Observing SATellite
FDR4ATMOS	Fundamental Data Record for ATMOSpheric Composition	GPP	Gross Primary Production
FIR	Far-Infrared electromagnetic spectrum	GRaCE	G-band Radar for Cloud Experiments
FIRMOS	Far-Infrared Radiation Mobile Observation System	GRASP	Generalized Retrieval of Aerosol and Surface Properties
FLEX	The FLuorescence EXplorer mission	GSG	GOME-SCIAMACHY-GOME-2
FLEXPART-WRF	FLEXible PARTicle dispersion model version that works with the Weather Research	GTO	ECV GOME-type Total Ozone Essential Climate Variable
	and Forecasting mesoscale meteorological model	H2020	European Union Horizon 2020 programme
FMI	Finnish Meteorological Institute, Finland	H20	Water Vapour
FOCAL	Fast atmOspheric traCe gAs retrieval	H20-IS0	Water Vapour Isotopologues
FORUM	Far-infrared Outgoing Radiation Understanding and Monitoring	HAPS	High Altitude Pseudo Satellite
FP_ILM	Full-Physics Inverse Learning Machine	HARPOL	Harmonizing and advancing retrieval approaches for present
FRESCO	Fast Retrieval Scheme for Clouds from the Oxygen A band		and future polarimetric space-borne atmospheric missions project
FRM4D0AS	Fiducial Reference Measurements for Ground-Based DOA S	НСНО	Formaldehyde
FTIR	Fourier Transform Infrared	HCI	Hydrochloric acid
GANs	Generative Adversarial Networks	HCN	Hydrogen cyanide
GAW	Global Atmosphere Watch Programme	HDO	Hydrogen-Deuterium Oxide
GE_LER	Geometry-dependent Effective Lambertian Equivalent Reflectivity	HERMES	High-Elective Resolution Modelling Emission System
GEISA	Gestion et Etude des Informations Spectroscopiques Atmosphériques database		of the Barcelona Supercomputer Centre
GEMS	Geostationary Environment Monitoring Spectrometer	HITRAN	HIgh resolution TRANsmission molecular spectroscopic database



HOCI	Hypochlorous acid
HSBB	Hemispherical Blackbody
IAGOS	In-service Aircraft for a Global Observing System
IASI	Infrared Atmospheric Sounding Interferometer
ICOS	Integrated Carbon Observation System network
IDPF-S	Instrument Data Processing Facility – Sounder
ILW	Integrated Liquid Water
INGV	National Institute of Geophysics and Volcanology, Italy
INOE	National Institute of Research and Development for Optoelectronics, Romania
IR	Infra-Red electromagnetic spectrum
JATAC	Joint Aeolus Tropical Atlantic Campaign
JAXA	Japan Aerospace Exploration Agency, Japan
KIT	Karlsruhe Institute of Technology, Germany
KLIMA	Kyoto protocoL Informed Management of the Adaptation
KNMI	Royal Netherlands Meteorological Institute, Netherlands
L2PF	Level-2 Processing Facility
Landsat	The NASA/USGS Program that provides space based records of Earth's land data
LEO	Low Earth Orbit
LER	Lambertian-equivalent reflectivity
LGBM	Light Gradient Boosting Machine
LIDAR	Light Detection And Ranging
LOTUS	Long-term Ozone Trends and Uncertainties in the Stratosphere
LSR	Lidar Surface Returns
MAMAP	Methane Airborne MAPper
MAP	Multi-Angle Polarimetric instrument
MAX-	Multi-Axis
MAX-DOAS	Multi Axis Differential Optical Absorption Spectroscopy
MERIS	Medium Resolution Imaging Spectrometer

MetOp	Meteorological Operational Satellites		
MetOp-SG	Meteorological Operational Satellites - Second Generation		
MEGRIDOP	MErged GRIdded Dataset of Ozone Profiles		
MFASIS	Method for FAst Satellite Image Synthesis		
MIPAS	Michelson Interferometer for Passive Atmospheric Sounding		
MIR	Mid-InfraRed electromagnetic spectrum		
MLE	Maximum Likelihood Estimation		
MLS	Microwave Limb Sounder		
MODIS	Moderate Resolution Imaging Spectroradiometer		
MOOC	Massive On-line Courses		
MPI	Max Planck Institute, Germany		
MPIC	Max Planck Institute for Chemistry, Germany		
MSI	Multi-Spectral Imager		
MTG-S	Meteosat Third Generation Sounder		
MUSES	MUltiSpEctra, MUlti-SpEcies, MUlti-Sensors		
MUSICA	MUlti-platform remote sensing of Isotopologues for investigating		
	the Cycle of Atmospheric water		
MW	MicroWave		
NASA	National Aeronautics and Space Administration, US		
NASA/GSFC	National Aeronautics and Space Administration Goddard Space Flight Center, US		
NASA/JPL	National Aeronautics and Space Administration Jet Propulsion Laboratory, US		
NATALI	Neural Network Aerosol Typing Algorithm		
NDACC	Network for the Detection of Atmospheric Composition Change		
NDSA	Normalised Differential Spectral Attenuation		
NEWIUN	Improving dust monitoring and forEcasting through Aeolus Wind data assimilation pr		
NH3			
NIES	National Institute for Environmental Studies		
NILU	Norwegian Institute for Air Research, Norway		



NITROSAT	Earth Explorer 11 mission candidate
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- **NIR** Near-Infrared electromagnetic spectrum
- **NMVOCs** Non-Methane Volatile Organic Compounds
 - NN Neural Network
 - **NO2** Nitrogen dioxide
 - **NOA** National Observatory of Athens, Greece
 - NW North-West
 - **O3** Ozone
 - **OCIO** Chlorine dioxide
 - **OCO** Orbiting Carbon Observatory
 - **OCRA** Optical Cloud Recognition Algorithm
 - **OLCI** Ocean and Land Colour Instrument
 - **OMI** Ozone Monitoring Instrument
- **OMPS** Ozone Mapping and Profiler Suite
- **OSIRIS** Origins, Spectral Interpretation, Resource Identification, Security, Regolith Explorer
 - **PAL** Product Algorithm Laboratory
 - PAN Peroxyacetyl nitrate
- **PARASOL** Polarization & Anisotropy of Reflectances for Atmospheric Sciences coupled with Observations from a Lidar
 - **PCSF** Potential Cloud Shadow Flag
 - **PDAP** Payload Data Acquisition and Processing
 - **PGN** Pandonia Global Network
 - **PM2.5** Particulate Matter of 2.5 micrometers or below
 - **PM10** Particulate Matter of 10 micrometers or below
- **PRISMA** PRecursore IperSpettrale della Missione Applicativa
 - **PSC** Polar Stratospheric Cloud
 - **QA** Quality Assurance
- **QA4ECV** Quality Assurance for Essential Climate Variables project

QA4EO	Quality Assurance Framework for Earth Observation		
R&D	&D Research and Development		
RADAR	Radio Detection and Ranging		
RAL	Space STFC, UK		
REFIR-PAD	Radiation Explorer in the Far InfraRed – Prototype for Applications and Development		
RemoTAP	Remote Sensing of Trace gases and Aerosol Properties		
RF	RadioFrequency		
ROCINN	Retrieval of Cloud Information using Neural Networks		
RTOA	Reflectance at the Top of the Atmosphere		
SABER	Sounding of the Atmosphere using Broadband Emission Radiometry instrument		
SACR	Simultaneous Atmospheric and Cloud Retrieval		
SATCROSS	Satelliti CoROtanti per la Stima di vapor acqueo in tropoSfera		
SBUV	Solar Backscatter Ultraviolet observing system		
SCA	Standard Correct Algorithm		
SCD	Slant Column Density		
SCIAMACHY	SCanning Imaging Absorption spectroMeter for Atmospheric CartograpHY		
Sentinel5-P	Sentinel5 Precursor		
STFC UKRI	Science and Technology Facilities Council, UK		
SHADOZ	Southern Hemisphere Additional Ozonesondes		
SIC	Sea Ice Concentration		
SIF	Solar Induced Fluorescence		
SLSTR	Sea and Land Surface Temperature Radiometer		
SNR	Signal to Noise Ratio		
S02	Sulphur dioxide		
SO2-LH	Sulphur dioxide layer height		
SRFP SRON	Full Physics algorithm		
SRON	Netherlands Institute for Space Research, The Netherlands		
SSA	Single Scattering Albedo		



SSMIS	Special Sensor Microwave Imager Sounder
SUOMI-NPP	Suomi National Polar-orbiting Partnership
SWIR	Short-wave infrared electromagnetic spectrum
SZA	Solar Zenith Angle
TAFTS	Tropospheric Airborne Fourier Transform Spectrometer
TanSat	Chinese Carbon Satellite
ТСС	Total Cloud Cover
TCCON	Total Carbon Column Observing Network
TCWV	Total Column Water Vapour
TEMPO	Tropospheric Emissions: Monitoring of Pollution
TIMED	Thermosphere Ionosphere Mesosphere Energetics Dynamics satellite
TIR	Thermal Infrared electromagnetic spectrum
ΤΟΑ	Top Of Atmosphere
TOAR	Tropospheric Ozone Assessment Report
ТОС	Total Ozone Column
TOPAS	Tikhonov regularised Ozone Profile retrievAl with SCIATRAN
TPM	Third Party Mission
TROPESS	TRopospheric Ozone and its Precursors from Earth System Sounding
TROPOMI	Tropospheric Monitoring Instrument
TROPOS	Leibniz Institute for Tropospheric Research, Germany
TROPOSIF	S5P+ Innovation project for Solar Induced Chlorophyll Fluorescence retrieval from
	TROPOMI
TRUTHS	Tracebla Radiometry Underpinning Terrestrial - and Helio - Studies
TUT	Turnover times
UCL	University College London, UK
UKESM	The UK Earth System Model project
UoB	University of Bremen, Germany
UoL-FP	University of Leicester Full Physics retrieval algorithm, UK

UPV	Universitat Politecnica de Valencia, Spain
USASK	University of Saskatchewan, Canada
UTLS	Upper Troposphere/Lower Stratosphere
UV	Ultra Violet electromagnetic spectrum
UVNS	UV/VIS/NIR/SWIR
UV/VIS	Ultraviolet-visible electromagnetic spectrum
VAO	Virtual Alpine Observatory
VCAL	Vicarious Calibration portal
VCD	Vertical Column Density
VDAF	Validation Data Analysis Facility
VDAF-AVS	Validation Data Analysis Facility Automated Validation Server
VIIRS	Visible Infrared Imaging Radiometer Suite
VIPR	Vapor In-cloud Profiling Radar
VIS	Visible electromagnetic spectrum
VOC	Volatile Organic Compounds
WFM-DOAS	Weighting Function Modified Differential Optical Absorption Spectroscopy
WMO	World Meteorological Organisation, Switzerland
WIVERN	Wind Velocity Radar Nephoscope mission
WOUDC	World Ozone and Ultraviolet Radiation Data Centre
WRF	Weather Research and Forecasting model
WRF-	Chem Weather Research and Forecasting model coupled with Chemistry
WV-3	WorldView-3 satellite
XCO2	column-averaged mixing ratio of carbon dioxide
XLH4	column-averaged mixing ratio of methane
XGB00St	Random Forest and Extreme Gradient Boosting machine learning model
XH2U	column-averaged mixing ratio of water vapour
XN2U	column-averaged mixing ratio of hitrous oxide
ZSL	Zenith-Sky scattered Light



3. Objectives, Themes, Scientific Committee and Session Chairs

The science objectives of ATMOS-2021 were

- Provide a platform for scientific exchange and to assess the state of the art of atmospheric applications;
- Foster the scientific community in atmospheric research;
- Present mission status, algorithms, and products for the currently operating Copernicus Sentinel-5P and Aeolus missions;
- Provide updates on activities regarding ESA Third Party missions;
- Demonstrate the synergistic use of different atmospheric instruments;
- Present scientific results related to the Copernicus Atmospheric Services CAMS & C3S;
- Discuss novel atmospheric mission, instrument and algorithm concepts, e.g., Scout Missions, SmallSats, constellations, HAPS, miniaturisation, AI algorithms;
- Provide a forum for scientists to formulate community recommendations.

Provide updates on development and science activities regarding future missions, e.g Copernicus Sentinel-4, Copernicus Sentinel-5, Copernicus CO2M, FORUM, EarthCARE, Altius, FLEX, TRUTHS and HARMONY

Present large-scale international initiatives to support the R&D activities relevant to atmosphere satellite missions and promote synergy with Copernicus Sentinels, Earth Explorers, and other missions;

Review and assess the progress according to the recommendations of the ESA ATMOS-2018 Atmospheric Science Conference (http://atmos2018.esa.int/page_atmos2018 report.php);







3. Objectives, Themes, Scientific Committee and Session Chairs

The Conference focused around the following themes

- Reactive trace gases in the atmosphere;
- Clouds and aerosols;
- Anthropogenic greenhouse gases;
- Biogenic sources of greenhouse gases;
- Volcanic emissions;
- Solar induced fluorescence;
- Water vapour;
- Air quality and climate monitoring from space;
- Stratospheric and middle-atmosphere processes;
- Atmospheric dynamics;
- Earth's radiation budget;
- Results on the generation of atmospheric Essential Climate Variables;
- Atmospheric applications and service development;
- Data assimilation and forecasting;
- New and innovative technologies for atmospheric remote sensing;
- Synergy with other Copernicus Sentinels, ESA Earth Explorers and other missions.

The organising committee consisted of

Christian Retscher (ESA/ESRIN), Claus Zehner (ESA/ESRIN), Thorsten Fehr (ESA/ESTEC), Simon Pinnock (ESA/ECSAT), Diego Fernandez (ESA/ESRIN)





The Scientific Committee consisted of

Ilse Aben (SRON), Dimitris Balis (AUTH), Hartmut Boesch (University of Leicester), Helen Brindley (Imperial College London), Dominik Brunner (EMPA), Michael Buchwitz (University of Bremen), Carlo Buontempo (ECMWF), John P. Burrows (University of Bremen), Andre Butz (University of Heidelberg), Alexander Cede (LuftBlick), Ugo Cortesi (CNR), David Crisp (NASA/JPL), Doug Degenstein (USASK), Oleg Dubovik (University of Lille/CNRS), Didier Fussen (BIRA-IASB), Frank Hase (KIT), Anthony Illingworth (University of Reading), Brian Kerridge (SFTC UKRI), Ruediger Lang (EUMETSAT), Barry L. Lefer (NASA/GSFC), Yi Liu (CAS), Diego Loyola (DLR), Doina Nicolae (INOE), Vincent-Henri Peuch (ECMWF), Caroline Poulson (Bureau of Meteorology), Oliver Reitebuch (DLR), Andreas Richter (University of Bremen), Philipp Schneider (NILU), Ad Stoffelen (KNMI), Johanna Tamminen (FMI), Michel Van Roozendael (BIRA-IASB), Pepijn Veefkind (KNMI), Thomas Wagner (MPI), Kaley Walker (University of Toronto)

The sessions were co-chaired by

non-ESA chairs:

Ilse Aben (SRON), Holger Baars (TROPOS), Frank Baier (DLR), Richard J. Bantges (Imperial College London), Hartmut Boesch (University of Leicester), Helen Brindley (Imperial College London), Dominik Brunner (EMPA), Michael Buchwitz (University of Bremen), Carlo Buontempo (ECMWF), John P. Burrows (University of Bremen), Alessandra Cacciari (EUMETSAT), Stefano Corradini (INGV), Ugo Cortesi (CNR), Doug Degenstein (University of Saskatchewan), Oleg Dubovik (University of Lille), Federico Fierli (EUMETSAT), Daniele Gasbarra (Shamrock Space Services c/o ESA-ESRIN), Sebastian Gimeno Garcia (EUMETSAT), Anthony Illingworth (University of Reading), Rigel Kivi (FMI), Alexander Kokhanovsky (TeleSpazio Belgium), MariLiza Koukouli (AUTH), Natalya A. Kramarova (NASA/GSFC), Isabell Krisch (DLR), Ruediger Lang (EUMETSAT), Rasmus Lindstrot (EUMETSAT), Hannakaisa Lindqvist (FMI), Diego Loyola (DLR), Marta Luffarelli (Rayference), Ronny Lutz (DLR), Doina Nicolae (INOE), Vincent-Henri Peuch (ECMWF), Thomas Popp (DLR), Caroline Poulsen (Bureau of Meteorology, Australia), Fred Prata (AIRES Pty Ltd), Oliver Reitebuch (DLR), Andreas Richter (University of Bremen), Michel van Roozendael (BIRA-IASB), Philipp Schneider (NILU), Richard Siddans (RAL), Viktoria Sofieva (FMI), Gabriele P. Stiller (KIT), Nicolas Theys (BIRA-IASB), Martin Tiefengraber (LuftBlick), Tim Trent (University of Leicester), Pepijn Veefkind (KNMI), Kaley Walker (University of Toronto)

ESA chairs:

Angelika Dehn (ESA/ESRIN), Thorsten Fehr (ESA/ESTEC), Yasjka Meijer (ESA/ESTEC), Hilke Oetjen (ESA/ESTEC), Simon Pinnock (ESA/ECSAT), Christian Retscher (ESA/ESRIN), Anne Grete Straume (ESA/ESTEC), Claus Zehner (ESA/ESRIN)













4. Plenary Sessions Summary & Highlights

4.1 Science from Space & Current Missions

After some introductory remarks by ESA, an overview of the societal applications of atmospheric remote sensing has been given in a keynote address by FMI. Satellites have a key role in the monitoring and the evolution of ozone as demonstrated by the support of remote sensing measurements to the Montreal protocol in terms of ozone recovery. Satellite observations are becoming more crucial in supporting air quality monitoring strategies thanks to the gradual increase of the spatial and temporal resolution. Remote sensing products are widely used also for health applications such as UV radiation and pollutants exposure. Another fundamental application is related to the top-down emission estimates that are needed for verifying and improving emission inventories and the understanding of the spatial distribution of emissions.

The status of the Copernicus Sentinel-5P mission was presented by ESA. The mission was launched in October 2017 and is in routine operation since March 2019 providing 250 TByte of data to the user community daily. Approximately 90% of the Level 2 near-real time (NRT) data is provided after 2 hours of sensing and Level 1 data after six hours, respectively. Many examples of successfully using TROPOMI observations like the monitoring of the ozone layer, the decrease of air pollution during the Covid-19 pandemic and the vegetation-fire emissions in Australia have been presented. New products such as ozone profile and improved methane, formaldehyde and sulphur dioxide products will be released in the course of 2022. The improved Level 1 product includes degradation correction for radiances. Following the release a reprocessing campaign for all Level 2 products will be performed. Nine new Sentinel-5P prototype products (CHOCHO, OCIO, H₂O-ISO, SO₂-LH, AOD/BRDF, SIF from Innovation



Sentinel-5 Precursor and Aeolus are the ESA missions related to the detection of trace gases such as nitrogen dioxide, ozone, formaldehyde, sulphur dioxide, methane, carbon monoxide and aerosols and for measuring wind profiles from space.







projects and H₂O, BrO from PAL project) are under finalisation and the upgrades to preoperational product is starting with Sentinel-5P PAL (Product Algorithm Laboratory). After the pre-operational product demonstration via PAL new Sentinel-5P core products can be proposed to the European Commission. Finally, a consistent NO₂ dataset is available to the user community from December 2021 processed at PAL.

Further, the status of ESA's Aeolus wind mission was presented. The scientific objectives of the mission are related to the improvements of the quality of weather forecasts and to advance our understanding of atmospheric dynamics and climate processes. The satellite performs well and within specifications, with a data acquisition rate of >98%. The UV Laser energy is stable at about 70 mJ and after a forced switch of the instrument to survival mode in October 2021 due to software issues, instrument operation has resumed nominally. Investigations are ongoing to mitigate the continuous loss of atmospheric return signals. Thanks to algorithm developments, random errors of Aeolus products are slowly decreasing and also the bias has improved. The Level-2A product is now mature and has been released in summer 2021. A statistically significant positive impact of Aeolus observations assimilation has been seen by ECMWF and MetOffice. Other case studies such as Aeolus observations of atmospheric gravity waves and long-range transport of aerosols from forest fires have been presented.

Results from using Sentinel-5p and Aeolus data are discussed in later sections.

4.2 Copernicus Services & Trainings

The status of the Copernicus Climate Change Service (C3S) has been discussed. C3S supports 22 Essential Climate Variables (ECVs) in five thematic areas: atmospheric physics, atmospheric

Atmos 2021 – Conference Report and User Recommendations



Copernicus is the European Union's Earth observation programme, looking at our planet and its environment to benefit all European citizens. It offers information services that draw from satellite Earth Observation and in-situ (non-space) data. Vast amounts of global data from satellites and ground-based, airborne, and seaborne measurement systems provide information to help service providers, public authorities, and other international organisations improve European citizens' quality of life and beyond. The information services provided are free and openly accessible to users.







composition, ocean, land hydrology & cryosphere, and land biosphere. All variables are available with co-organized also with specific sessions during conferences such as EGU. Beyond the school activities long term and consistent time series that are constantly updated. A new set of web-based tools have other initiatives like Massive On-line Courses (MOOC) have been organised. The latest iterations were on been developed for the monitoring of climate change. This allows users to generate, in a traceable Artificial Intelligence for Earth Monitoring organised by Copernicus and on air quality monitoring during and reproducible way, Climate Indicators. These enable an operational monitoring on the long term Covid-19 organised by ESA. Other provided training formats relate to thematically focused workshops evolution of several key variables used to assess the global and regional trends of warming climate such such as the training schools on dust aerosol detection held in November 2021. as temperature, sea ice and greenhouse gas concentrations and fluxes. Future reanalysis by means of ERA6 will have a better representation of key atmosphere-ocean processes and feedback thanks to the 4.3 International Satellites, Missions and Products enhanced ocean and land data assimilation.

NASA provided an overview of its latest developments regarding trace gases observations. A worldwide CAMS combines information from Earth observation satellite and in-situ measurements, these inputs are large decrease of NO₂ and SO₂ concentrations between 2005 and 2019 has been assessed by means of processed using numerical models at global and regional scale and the outputs are provided to a wide Ozone Monitoring Instrument (OMI) observations. A new series of products related to Volatile Organic range of users, from policy sector to commercial sector and air quality applications. Recently CAMS data Compounds (VOC) such as isoprene and a new ammonia product were retrieved in the IR band from IASI has also been taken up by smartphone applications endorsed by the World Meteorological Organisation observations. The future geostationary mission TEMPO for the monitoring of atmospheric composition (WMO) and the European Environment Agency (EEA). CAMS has been renewed for another 7 years until over North America and a dedicated validation campaign using also TEMPO simulated data held in 2028 and will increase the collaboration with the member states providing new outputs related to September 2021 have been presented. pollutants and greenhouse gas fluxes. From October 2021, CAMS is assimilating tropospheric TROPOMI NO₂ measurements using also chemistry to account for the large NO₂ diurnal variability. The impact of JAXA gave an overview of GOSAT and GOSAT-2 CO_2 measurements covering a total of twelve years of operation in space. Monthly maps of XCO₂, XCH₄, AOD and SIF are available from the JAXA website. During the Covid-19 pandemic these observations were provided to the trilateral ESA/NASA/JAXA

this assimilation on surface NO₂ is small but reduces the NO₂ bias over China. The assimilation of SO2 layer height data from TROPOMI for large volcanic eruptions is in a test phase showing an improved agreement between IASI and CAMS plume altitude if TROPOMI data are ingested. EO-dashboard (https://eodashboard.org/) in which the level of pollutants and greenhouse gases over 50 world megacities have been monitored. The Vicarious Calibration portal (VCAL) for greenhouse An overview of the training activities co-organized by ESA, EUMETSAT and ECMWF/CAMS has been gas sensors has been introduced. Access to resources on the portal is free of charge and provides presented. The so-called Joint Training on Atmospheric Composition provides lectures from top level methodologies of vicarious calibration for various size footprint and off-nadir data, 13-year annual scientists and hands-on support on dealing with atmospheric data. During the school events participants joint campaign data for Cal/Val and analytical results from various types of spectrometer such as are encouraged to develop their own projects centred on the practical use of Copernicus (and related) GOSAT FTS, OCO and TROPOMI. In order to improve the estimates of global and local fluxes, JAXA data. Since 2019 more than 15 events (some organised only by EUMETSAT and ECMWF) have been developed a new imaging spectrometer for air-borne observations. Currently this is used on passenger



aircrafts allowing the characterization of plumes producing fine scale CO₂ and NO₂ maps.

The new XCO₂ dataset from TanSat has been introduced by CAS. These data have been coupled with TROPOMI NO₂ observations in order to detect anthropogenic emissions. TanSat data can be downloaded from e.g. the ESA Third Party Mission (TPM) webpage: https://tpm-ds.eo.esa.int/oads/access/.GlobalCO, flux maps have been produced using the new dataset showing a large reduction of the fluxes uncertainties with respect to the previous version. A novel satellite, named GaoFen-5, launched in 2021 has been presented. It consists of two land imagers and five atmospheric sounders, one specifically for the retrieval of greenhouse gases. The next generation of TanSat will be a constellation of three satellites able to measure CO₂, NO₂, CH₄, CO and SIF with a daily global coverage and a spatial resolution of 2x2 km² that can be increased to 500x500 m² in target mode.

The first year of air quality observation from the Korean Geostationary Environment Monitoring Spectrometer (GEMS) over Asia was presented by the GEMS Science Team. GEMS provides hourly observations of O₃, NO₂, SO₂, HCHO, CHOCHO, AOD, AAI with spatial resolution of 3.5x8 km². The instrument was launched in February 2020, with daily operation having started in April 2020. The satellite is planned to be in operation for over 10 years. First validation results related to the period August-October 2020 and April-July 2021 were presented. A good agreement with AERONET, OMI and TROPOMI observations was found. Thanks to the hourly observation capability, GEMS was able to detect daily ozone dynamics and a dust plume intrusion related to the Siberian wildfire over Asia.

In August 2021, the Canadian-led Atmospheric Chemistry Experiment (ACE) mission completed its eighteenth year in orbit on board the SCISAT satellite. The long lifetime of ACE-FTS is providing a valuable time series of composition measurements that contribute



The tri-agency COVID-19 Dashboard (https://eodashboard.org/) is a concerted effort between the European Space Agency (ESA), Japan Aerospace Exploration Agency (JAXA), and National Aeronautics and Space Administration (NASA). The dashboard combines the resources, technical knowledge and expertise of the three partner agencies to strengthen our global understanding of the environmental and economic effects of the COVID-19 pandemic.







to our understanding of ozone recovery, climate change and pollutant emissions. A comparison between the lower part of ozone vertical profiles and ozone sondes has been carried out showing good agreement in upper troposphere/lower stratosphere (UTLS) with an increase of the absolute difference in the stratosphere. Different retrievals from ACE-FTS such as HCl, CLONO₂, HOCl and ClO have also been used to develop a climatology for inorganic chlorine (Cly) that was compared with CMAM-39 model simulations. This shows an underestimation of the model at both mid and high Northern latitudes during winter while a good agreement was found outside of polar winter and spring. A new comparison between ACE-FTS and MIPAS chloro-fluoro-carbon (CFC) measurements between 2005 and 2012 showed a typical difference around 10% with MIPAS 10-20 pptv higher than ACE-FTS.

4.4 Future Missions – Copernicus Sentinels

The upcoming Sentinel-4 mission will consist of a UV/Vis/NIR (UVN) imaging spectrometer being part of the geostationary Meteosat Third Generation - Sounder (MTG-S) mission. The planned lifetime is about 15 years with two Sentinel-4 instruments operated in sequence. The mission will allow air quality monitoring over Europe with hourly coverage. The launch is expected in the first quarter of 2024. ESA will cover the mission operation until the end of commissioning and EUMETSAT will be responsible for routine operation. The list of operational Level 2 Copernicus products consists of O_3 , NO_2 , HCHO, CHOCHO, SO_2 , clouds and aerosols complemented by the operational AC-SAF products SO2 layer height and H₂O. Algorithms are already verified on synthetic data and the next steps will be the testing with proxy data from other geostationary missions like GEMS. The Sentinel-4 Level 1 Operational Processor is under development as part of the MTG Instrument Data Processing Facility - Sounder (IDPF-S) ground segment, while the Level 2 Processor (ESA/DLR development) is integrated into the MTG Level-2 Processing Facility (L2PF).



The Copernicus Carbon Dioxide Monitoring mission, or CO2M for short, is one of Europe's Copernicus Sentinel Expansion missions and will be the first to measure how much carbon dioxide is released into the atmosphere specifically through human activity





Sentinel-5 will follow the heritage of Sentinel-5P allowing the observation of atmospheric composition with a daily global coverage. The instrument consists of a UV/Vis/NIR/SWIR (UVNS) imaging spectrometer. The planned mission lifetime is 21 years with three Sentinel-5/UVNS in sequence and will be operated by EUMETSAT. The launch is expected for the second quarter of 2024. Level-2 products cover the same Sentinel-4 compounds with the addition of CO and CH₄. Algorithms are already tested and verified with both synthetic and real data, while the uncertainty budget per product is established. Possible future improvements on algorithms testing can be based on Sentinel-5P experience. Sentinel-5 Level 1 and Level 2 Operational Processors are implemented in EPS-SG Payload Data Acquisition and Processing (PDAP) facility. For both missions a joint ESA/EUMETSAT calibration and validation plan is already prepared and will involve ground-based observations from NDACC, Pandonia, WOUDC, Eubrewnet, and TCCON networks and satellite data from GOME-2, Sentinel-5P, TEMPO, GEMS while CAMS will be used for model-based validation.

The launch of CO2M for the monitoring of anthropogenic CO₂ is expected for 2025. The overall mission requirements are the detection and the monitoring of emitting hot spots such as megacities or power plants which require high precision data, high spatial resolution and frequent revisit to quantify the emissions. Other requirements are related to the assessment of emission changes against local reduction targets which shall have no regional biases and no long-term drifts. The instrument consists of a pushbroom imaging spectrometer characterised by a 250 km swath width with four bands: Vis (405-490 nm), NIR (747-773 nm), SWIR-1 (1590-1675 nm) and SWIR-2 (1990-2095 nm). Currently operating CO₂ missions filter out data for AOD>0.3, while CO2M will use a light path correction by measuring effective aerosol and clouds allowing measurements with higher aerosol loading (at least for AOD<0.5) and with higher accuracy also over regions characterised by high AOD. In order to avoid cloud contamination, a cloud imager with three different bands is able to detect both lower water clouds and cirrus. CO2M will provide CO₂, CH₄, NO₂ and SIF measurements with a 2x2 km² spatial resolution and aerosols with $4x4 \text{ km}^2$.

For CO2M, the availability of robust and well-maintained ground-based and in-situ networks, complemented by model data and relevant operational satellite data from other missions will be of vital importance for monitoring and maintaining the stringent long-term performance requirements of the mission. Continuous operational monitoring, verification and validation systems - relying on robust data-streams from many different sources - might be established in close collaboration with our European partner agencies and the networks of ground-based remote-sensing greenhouse-gas measurement stations.

4.5 Future Missions – Earth Explorers & Earth Watch

The ALTIUS mission consists of a limb sounder for the monitoring of stratospheric ozone at relatively high vertical resolution of around 3.5 km. Today only a few missions provide limb measurements, several might terminate within the next few years, consequently ALTIUS will fill an upcoming data gap. ALTIUS observations will contain several snapshots at different wavelengths taken by three separated cameras in the UV, Vis and NIR range. The innovative concept of the ALTIUS mission relates to the multimode observations that allows the instrument to perform in limb scattering, but also in solar, lunar, stellar and planetary occultation mode. A full orbit of ALTIUS will consist of limb observations coupled with occultation observations on the dark side of the orbit. The instrument configuration has been modified due to technical and programmatic trade-offs on the original SWIR channel. This led to the adoption of a 600-1020nm NIR channel. A further trade-off relates to the spectral range versus improved resolution for allowing NO₂ retrievals and a trade-off of spectral range versus spectral leak rejection. About 20% of mission time will be used for calibration and dedicated observations. The launch is foreseen for May 2025, and after satellite commissioning an operational phase of three years is expected, possibly extended to five years.

The launch of the EarthCARE mission is expected for the year 2023 (date is subject to change based on the availability of launch capabilities). The mission will address the impact of clouds and aerosols



on radiation, observing cloud and aerosol profiles, precipitation and broad-band solar and thermal radiation. The payload will consists of four instruments: a Cloud Profiling Radar (CPR) handled by JAXA that will provide vertical profiles of thick clouds and precipitation products, an Atmospheric LIDAR (ATLID) that will provide vertical profiles of thin clouds and aerosols products, a Multi-Spectral Imager (MSI) for retrieving cloud and aerosol information and a Broad-Band Radiometer (BBR) to detect top of atmosphere (TOA) short/long wave radiances and flux. Synergistic retrievals such as cloud/precipitations/aerosols vertical profiles, 3D cloud and aerosol scenes and a second TOA radiances and fluxes product are expected. The total data volume will be around 70 GB per orbit with a data latency of ~5.5 hours from sensing. Products from LIDAR and cloud Radar will be assimilated into the operational ECMWF model in order to improve the model performances on evaluation of clouds and precipitation.

The FORUM mission is discussed in a dedicated section below.

4.6 Future Missions – Earth Explorers Candidates

This section summarises latest developments on the three ESA Earth Explorer 11 candidate missions, which are related to monitoring the atmosphere.

The Changing Atmosphere InfraRed Tomography Explorer (CAIRT) aims to address changes in atmospheric circulation and transport, mixing processes, and their impact on atmospheric composition and surface climate. Some examples were discussed such as the relation between a weak polar vortex and the presence of Australian hot and dry extreme events. The main objectives of the mission relate to the detection of circulation between upper troposphere and lower stratosphere by means of accurate observations of age-of-air, temperature and trace gas concentrations and the impact of stratosphere-troposphere exchanges on tropospheric

Atmos 2021 – Conference Report and User Recommendations

EarthCARE will employ high-performance lidar and radar technology that has never been flown in space before, with the objective to deliver unprecedented datasets to allow scientists to study the relationship of clouds, aerosols and radiation at accuracy levels that will significantly improve our understanding of these highly variable parameters



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composition. The mission also aims to attribute changes in stratospheric ozone due to circulation and chemistry, quantify the flux of reactive nitrogen species from the upper atmosphere into the stratosphere and to detect aerosol composition and precursor gases. This will be achieved by means of infra-red limb imagery with a spectral coverage between 710 and 2200 cm-1 and a nominal sampling of 50x50 km². CAIRT will be the first infrared imaging limb sounder in space. A combination of CAIRT observations with nadir viewing instruments such as IASI and Sentinel-5 will allow the limb-nadir matching of the measurements improving the knowledge of the troposphere.

The primary objective of the Wind Velocity Radar Nephoscope (WIVERN) mission is the detection of global in-cloud winds using cloud particles as a tracer while the secondary objectives relate to the quantification of rainfall, snow, cloud water content and cloud depth. The payload consists of 94 GHz Doppler Radar orbiting at a height of 500 km able to complete a rotation in five seconds with an 800 km wide ground track. The Radar will transmit closely spaced pulse pairs polarised in the horizontal and vertical to achieve the high folding velocity needed to measure winds.

NITROSAT is a satellite mission concept for mapping reactive nitrogen at high horizontal resolution. The scientific motivation beyond this mission is to monitor nitrogen emissions, especially in the form of NOx and NH₃. Nowadays a lot is known on reactive nitrogen at the regional scale while there is a gap of knowledge on the landscape scale: local emissions cannot be monitored from space and cluster emission data cannot be disentangled easily. NITROSAT will provide measurements at sub-km scale allowing the disentangle of different sectors of emissions and assessing the impact of nitrogen deposition locally. This will support the implementation of strategies for nitrogen management. Specific mission objectives include the quantification of NO₂ and NH₃ emissions and their temporal patterns, the impact of these

Atmos 2021 – Conference Report and User Recommendations



The three ESA Earth Explorer candidate missions to be launched in the next years.





emissions on air quality and constrain the impacts on ecosystems of nitrogen dispersion and surface deposition. The payload will consist of a infrared imaging Fourier transform spectrometer for NH_3 and a visible imaging pushbroom spectrometer for NO_2 with a spatial resolution at least of 0.5x0.5 km².

4.7 The FORUM Mission

The FORUM mission will provide a highly accurate global dataset of spectrally resolved farinfrared radiances and will evaluate the role of the far-infrared in shaping the current climate, reducing the uncertainties in prediction of future climate change. The launch is expected in 2027 with 5 years of mission lifetime and FORUM will fly in loose formation with MetOp-SG-A. The payload will consist of a spectrometer with a spectral coverage of 100 to 1600 cm-1 with 0.5 cm-1 resolution. FORUM will be the first satellite able to measure far-infrared emissivity on a global scale and will provide a useful dataset to the Global Climate Model to detect changes in radiative surface temperatures. The far-infrared shows an enhanced sensitivity to ice cloud particle shape and can also provide very good information about cloud properties, but will also allow measuring the atmospheric water vapour content.

CNR-INO presented the Simultaneous Atmospheric and Cloud Retrieval (SACR) code, an algorithm comprising a forward and a retrieval model capable of simultaneously retrieving the main surface and atmospheric variables and the cloud optical and microphysical properties, from infrared spectral radiance measurements. In particular, the characterization of cirrus cloud radiative properties represents a paramount goal, since this type of clouds modulates the incoming solar radiation and the thermal outgoing emission from the ground. The procedure to retrieve relevant atmospheric parameters from FIR and MIR was presented by using simulated spectral radiances as those that will be measured by FORUM.

Atmos 2021 – Conference Report and User Recommendations



The FORUM mission will improve the understanding of our climate system by supplying most of the spectral features of the far-i contribution to the Earth's radiation, focusing particularly on water vapour, cloud properties and ice-snow surface emissivity.





An approach to calculate the spectral flux from the atmospheric state retrieved from the spectral radiance measurements was presented by CNR-INO. The atmospheric state (mainly, vertical profiles of humidity and temperature, and ozone column), cloud and surface properties are retrieved using an inversion model based on a line-by-line radiative transfer code and the retrieved parameters are then used to simulate the hemispherical spectral emission at the top-of-atmosphere. This approach was applied to one of the existing datasets acquired by stratospheric balloons covering the wide spectral range of FORUM. Results showed a good agreement with ERA5 long wave radiation flux.

In cold and dry conditions a significant fraction of the far-infrared (FIR) emission from the surface can reach the top of the atmosphere (TOA) influencing the radiation budgets of polar regions. The Far-Infrared Radiation Mobile Observation System (FIRMOS), a Fourier transform spectrometer, was built by CNR-INO as an instrument demonstrator for the future FORUM mission. The instrument was deployed for a ground-based campaign on Zugspitze (German Alps, 2962m a.s.l.) showing a good sensitivity in the 400-600 cm-1 range allowing the use of FIRMOS for future FORUM validation.

CNIT presented the outcomes of the SATCROSS project, a feasibility study for a space remote sensing system for the retrieval of tropospheric water vapour by means of a train of co-rotating low Earth orbit satellites (LEO). The approach is called NDSA (Normalised Differential Spectral Attenuation) method and is based on measuring the spectral sensitivity, which is the normalised incremental ratio of the spectral attenuation that was found to be linearly related to the integrated water vapour. It has been clarified that the method is not sensitive to the aerosols since liquid water has different features of absorption at these frequencies.

Atmos 2021 – Conference Report and User Recommendations



Aeolus is the first satellite mission to acquire profiles of Earth's wind on a global scale. These observations are being used to improve weather forecasts and climate models. The Aeolus satellite carries just one large instrument, a Doppler wind lidar that measure the winds sweeping around our planet.







4.8 Aeolus Mission Data Exploitation

The assimilation of Aeolus L2B wind profiles into numerical dispersion models has been successfully differences were reported for zonal bands with higher values at higher latitudes. tested for Etna volcanic eruptions. Simulations performed with the FLEXPART-WRF model with and without Aeolus assimilation showed a positive impact in monitoring and forecasting the dispersion of

Dust aerosols are a key component of the Earth-Atmosphere system with impacts on atmospheric volcanic ash when the model is initialised with Aeolus wind observations. processes, ecosystems and air quality. The core idea of the project ImproviNg dust monitoring and forEcasting through Aeolus Wind daTa assimilatiON (NEWTON) led by National Observatory of Athens (NOA), is to demonstrate the remarkable improvements on ECMWF numerical weather predictions attributed to Aeolus wind observations are being operationally assimilated by ECMWF and other meteorological services. Independent and high quality reference measurements are essential, as they permit the quantification the assimilations of Aeolus wind profiles. An analysis showed that for several cases, either with high of Aeolus wind biases. The Loon Balloon Network provides wind observations in the upper troposphere/ or low aerosol conditions, the WRF predictive skills were improved when the regional simulations were lower stratosphere which offer a valuable reference dataset for Aeolus product quality assessment in the initialised after the considerations of Aeolus wind assimilation. tropics. The comparison revealed a relatively good agreement on wind horizontal variability while for the KNMI showed how cloud and aerosol properties can be retrieved from the Atmospheric Laser Doppler vertical representativeness collocated radiosonde are needed.

In order to provide more data for the Aeolus validation, the Joint Aeolus Tropical Atlantic Campaign (JATAC) campaign has been conducted on Cabo Verde in July 2021. More than 35 flights with four aircrafts equipped with Doppler Aerosol Wind LIDAR (DAWN) were performed and 17 Aeolus orbits were underflown, four of these with a perfect collocation of Aeolus and the ground-based observations.

A combined aerosol AOD retrieval by using LIDAR surface returns (LSR) from Aeolus and collocated near surface wind speed estimates over ocean was presented by KNMI. The retrieval is based on the Aeolus wind measurements allow the derivation of atmospheric wave structures and wind gradients fundamental link between LIDAR surface returns, sea slope variance and near surface wind over water. above the oceans where the wind ground-based observations are sparse. DLR showed how the Aeolus Retrieved AOD from the LSR was compared with collocated L2A Aeolus operational extinction profiles detection of the planetary waves by means of the streamer events is a powerful instrument to infer obtaining a good agreement but showed a lower sensitivity than expected of LSR to near-wind speed and unexpected clear gradient between different land cover when LSR is averaged on a 1x1 degree grid. large-scale weather patterns.

ERA5 can produce very detailed information about the global dynamics without any gaps in the time series. The comparison between ERA5 and Aeolus revealed that Aeolus measurements are biased and Two algorithms of the Level 2A processor that aim to retrieve the atmospheric optical properties from the

Instrument (ALADIN) on board of Aeolus using an approach similar to the one deployed for ATLID (Atmospheric LIDAR), the LIDAR to be embarked on the Earth Clouds and Radiation Explorer (EarthCARE) future mission. Despite the low SNR ratio of the backscattered signals, comparison with CALIPSO and ground-based observations revealed the capabilities of Aeolus to detect aerosol and cloud properties.









Aeolus signal have been presented by CNRS. The Standard Correct Algorithm (SCA) does a direct retrieval of extinction and backscatter coefficients. LIDAR signals are processed to separate the contribution from molecules and particles called cross talk correction and the optical properties of the particles can be estimated from these cross-talk corrected signals and simulated molecular signals. The second algorithm called Maximum Likelihood Estimation (MLE) is able to determine a profile that optimally fits the signals while checking physical constraints (e.g. extinction not allowed to be negative and LIDAR ratio between 2 and 200sr) producing less sensitive results to the noise compared to SCA.

called Maximum Likelihood Estimation (MLE) is able to determine a profile that optimally fits the signals while checking physical constraints (e.g. extinction not allowed to be negative and LIDAR ratio between 2 and 200sr) producing less sensitive results to the noise compared to SCA. Recent research efforts have shown the potential of LIDAR backscatter to extract aerosol information providing insight on aerosol vertical structure. ECMWF presented results from the A3D project (Aeolus Aerosol Assimilation in the DISC) showing the technical feasibility of assimilating in-orbit data of particle backscatter from the ALADIN instrument. Aeolus L2A data have been used to demonstrate the positive impact of aerosol backscatter assimilation on the COMPO-IFS model.

4.9 Air Quality

KNMI presented the inversion algorithm Daily Emissions Constrained by Satellite Observations (DECSO) which can derive NOx emissions at 10-20 km resolution using TROPOMI observations. Emissions are divided in three categories: fossil-fuel, soil, and maritime emissions. Obtained emissions agree very well with HERMES and CAMS emission databases, only the seasonal variability of DECSO needs to be improved. A clear reduction of NOx emission was observed over cities in the European Union (EU) during the lockdown period in 2020 due to the Covid-19 pandemic.

FMI showed the capability of TROPOMI observations to detect single NO_2 plumes from container ships over the Mediterranean sea. The TROPOMI NO_2 value in the plume is defined as a mean of the three highest value NO_2 pixels that fall within a polygon, delimited by the ship's route for the past hour as well



The University of Edinburgh developed an analysis tool using a convolutional neural network (CNN) to identify plumes of NO_2 from TROPOMI data. Deep learning was trained using six thousand 28x28 pixel images of TROPOMI. More than 300,000 plumes were detected over power stations, oil and gas production areas and cities. NO_2 plumes from regions where inventories do not include emissions were found such as mid-Africa and Siberia. Few cases of false positives were detected and all scenes with cloud cover greater than 40% were discharged.

Remote sensing trace gases retrievals commonly assume horizontal homogeneity when computing the AMF with radiative transfer models. EMPA implemented a 3D box-AMFs to account for the effect of buildings in cities and applied it to NO_2 measurements from the airborne APEX spectrometer. Non-negligible 3D effects due to the slant geometrical path relate to image distortion of an emission plume and can result in a significant bias in emissions estimates. It was clarified that the dispersion model and the radiative transfer model use the same buildings map. The a-priori NO_2 distribution is impacted by buildings so a city-scale dispersion model is used to take these effects into account.



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MPI developed a method to retrieve the divergence of horizontal flux of trace gases by using TROPOMI NO₂ observations coupled with a wind field from ECMWF. The method works very well for point sources where spatial gradients of NO₂ are particularly high. More than 400 locations identified as NOx point sources have been detected. It was specified that the method looks not only on the top of the source but also in its proximity. Considering the derivative, both aerosols or lack of mixing cannot have a strong influence on the estimates. In the framework of the CitySatAir project, KNMI presented an integrated approach to monitor air quality at urban scale by means of satellite observations, ground-based stations and modelling. Urban emissions were estimated with high resolution urban-scale dispersion model assimilating data from satellite, city stations and low cost sensor networks. A geostatistical downscaling was developed to increase the spatial resolution of TROPOMI NO₂ observations for urban applications.

Column amounts of NO_2 variations over regions with strong responses to Covid-19 have been addressed by DLR using GOME-2 and TROPOMI NO_2 observations. Long term data sets were seasonally adjusted based on climatological seasonal variability and corrected for the wind speed. Drops in NO_2 were observed in China, US and Europe with a gradual rebounce corresponding to the recovery of social and economic activities.

Estimates of methane and nitrogen dioxide emissions from gas flaring and oil production activities in Russia by using TROPOMI, Sentinel-2 and VIIRS observations have been discussed by KNMI. Annual NOx emissions were derived from TROPOMI NO2 data using an exponentially modified Gaussian model while methane emissions were retrieved using the cross-sectional flux method. This approach works for gas flaring. Fugitive emissions cannot be detected. Emission estimates from satellites are higher compared to inventories, which underestimate the contribution from the oil and gas industry.



TROPOMI Sentinel-5P NO2 observations over Europe.







4.10 Ozone

A 25 years tropospheric ozone time series for the tropical band (20S to 20N) based on convective cloud Tropospheric ozone in discrete vertical layers was retrieved from OMI observations and compared with differential algorithm (CCD) was presented by DLR including data from SCIAMACHY, OMI, GOME-2A, UKESM1 simulations by University of Cambridge. Using the OMI dataset was possible to identify model GOME-2B, GOME-2C and TROPOMI. SCIAMACHY data are used as a reference and fitted as an offset and biases related to the differences between model and observations in lower stratospheric ozone trends. It a trend correction to the data of other sensors. From this long term dataset a mean tropical trend of was also possible to identify stratospheric transport of ozone into the troposphere as the main driver of 0.9 DU/decade in the tropospheric ozone was detected. A second data record that combines total ozone the North Atlantic ozone variability such as the Arctic oscillation. It was clarified that trend discrepancies columns from TROPOMI with BASCOE stratospheric ozone profiles has been presented. Both ozone between model and observations could be related to methane concentration variations. Methane is imposed in the model by observations, but the chemistry parameterization could have some missing datasets showed a very good agreement with significant trends over the ocean. Possible reasons for these trends relate to different albedo or to different cloud cover between continent and ocean. elements.

Another presentation from DLR showed global and regional ozone trends from the GOME-type Total UV satellite estimates of ozone are able to make high-quality estimates of stratospheric concentrations Ozone Essential Climate Variable (GTO-ECV) data record. GTO-ECV combines observations from a series of but tend to have lower performance in the troposphere. Thermal infrared (TIR) measurements exploit line pressure broadening to infer tropospheric ozone but typically do not perform as well in estimating six nadir-viewing satellite sensors of the GOME-type that measure in the ultraviolet and visible spectral range. GTO-ECV provides monthly mean total ozone at a remarkable spatial resolution of 1°x1°. In the stratospheric ozone. Large volumes of data are available from current satellite instruments such as OMPS framework of ESA-CCI+ it has been further improved and expanded with new satellite sensors including and TROPOMI in the UV, and AIRS and CrIS in the TIR, and ever-increasing amounts will be available from future instruments such as Sentinels 4, 5 and TEMPO (UV) and future iterations of CrIS (TIR). NASA/JPL TROPOMI on board Sentinel-5P. Spatial and seasonal distribution of trends and the correlation with presented the MUltiSpEctra, MUlti-SpEcies, MUlti-SEnsors (MUSES) retrieval algorithm being developed explanatory variables used in the regression model were presented, showing apparent signs of ozone for the TRopospheric Ozone and its Precursors from Earth System Sounding (TROPESS) framework. This recovery. algorithm has a flexible and generic Radiative Transfer model that covers the entire wavelength range from the UV to the TIR and a nonlinear optimal estimation retrieval algorithm. Using MUSES/TROPESS, University of Bremen presented global 03 trends from 1979 to 2020 using different merged total ozone datasets from satellite and ground-based observations. The merged datasets include data from NASA examples of multi-sensor retrievals of ozone from Suomi NPP CrIS and Sentinel-5P/TROPOMI were presented. The joint ozone retrieval was compared successfully with TROPOMI total and tropospheric MOD v8.7, NOAA Cohesive Data (COH) v8.7, Global Ozone Monitoring Experiment (GOME)-type Total column and similar agreement between CrIS-TROPOMI and CrIS-MLS retrieval is found for stratospheric Ozone (GTO-ECV), GOME-SCIAMACHY-GOME-2 (GSG) merged datasets (1995–2021) and the annual mean zonal mean data from ground-based measurements collected at the World Ozone and UV Data Centre profiles. It was clarified that the retrieval is not fully optimal at the moment, the TROPOMI-CrIS single profile retrieval takes about 10-15 minutes. (WOUDC). Trends showed a slow ozone recovery in both hemispheres, the median near global ozone







trend after 1996 was 0.5 ± 0.2 (2 σ) %/decade, which is in absolute numbers roughly a third of the decreasing rate of 1.4 ± 0.6 (2 σ) %/decade from 1978 until 1996. It was clarified that the improvement of ozone retrieval over polar regions can be very useful in the detection of the recovery trends.

The LOTUS community has recently concluded its revisit of long-term changes in stratospheric ozone in support of the upcoming 2022 WMO Ozone Assessment. BIRA-IASB presented updated estimates of trends in the vertical distribution of ozone between 2000 and 2020 and their coherence between data records and simulations by the Chemistry-Climate Model Initiative (CCMI). Positive trends of 1-4% dec-1 are found in the upper stratosphere depending on latitude, in good agreement with CCMI trends. For the lower stratosphere non-significant negative trends are found in the tropics and in the Northern hemisphere below 20 km, with larger discrepancies with CCMI trends. It was clarified that regarding the correlation matrix for trend uncertainties, for each climate data records the fit residuals for the 2000-2020 period were computed and after their correlations were evaluated.

At the University of Bremen ozone observations from two instruments with limb sounding capability, SCIAMACHY and OMPS-LP, were retrieved using the same radiative transfer model, spectroscopic databases and similar retrieval algorithms. The two datasets were merged to obtain a consistent time series of global O_3 distributions and were used to study long term ozone changes through the application of a multilinear regression over the period 2003-2020. Positive trends were found in the stratosphere at mid-latitudes with an increasing ozone concentration up to 2-4% per decade. Longitudinal asymmetries at Northern high latitudes in ozone trends have been highlighted in both satellite records especially during the winter semester with associated temperature trend asymmetries. Changes in meridional winds were also detected with an indication of a change in the strength and rotation of the

Atmos 2021 – Conference Report and User Recommendations



TROPOMI Sentinel5-p observation of ozone hole over Antarctica during 2020, one of the largest in recent years







have been presented showing very good agreement with ground-based observations and with TROPOMI stratospheric vortex. Simulations with the TOMCAT global 3-D chemistry transport model were carried out for the same period finding similarities and differences that can be explained considering specific and GOME-2 observations. dynamics processes.

BIRA-IASB presented an initial validation of the atmospheric ozone profiles retrieved from TROPOMI. FMI presented monthly 1x1 deg, global tropospheric ozone using a combination of total ozone columns The validation was carried out using a diagnostic dataset (DDS5) of fourteen preselected orbits that from OMI and TROPOMI with stratospheric ozone columns datasets from several available limbtogether collocate with more than one hundred ground-based correlative measurements. The validation viewing instruments. A method for data homogenization was set up, which includes the removal of methodology relied on the analysis of data retrieval diagnostics and on comparisons of TROPOMI data biases and a-posteriori estimation (validation) of random uncertainties, thus making the data from with ground-based measurements. The latter were acquired by ozonesondes, stratospheric ozone LIDARs, different instruments compatible with each other. The global distributions of tropospheric ozone exhibit and tropospheric ozone LIDARs. Preliminary results showed a slight striping along the orbit and a bias below 10% in the troposphere. enhancements associated with the regions of high tropospheric ozone production.

University of Bremen developed the TOPAS (Tikhonov regularised Ozone Profile retrievAl with SCIATRAN) algorithm to retrieve vertical ozone profiles from space-borne nadir UV radiance measurements. UoB presented a combined retrieval approach using UV band from TROPOMI and IR band from CrIS. The retrieved ozone profiles have an improved vertical resolution varying between 6 and 9 km in the stratosphere. Below 18 km the sensitivity is limited and the vertical resolution is reduced. The TOPAS ozone profiles were validated using collocated stratospheric ozone LIDAR and ozone-sonde measurements showing an improvement of UV+IR over UV-only retrieval.

A novel approach to retrieve total ozone columns (TOC) by using measurements in the visible spectrum Chappuis band (500-700 nm) was presented by Telespazio Belgium. This approach is based on the fact that the top-of-atmosphere reflectance observed over a highly reflective ground (snow, ice, deserts) has a minimum in the visible spectrum range, around 600 nm. The feature is due to the absorption of solar light by the atmospheric ozone. This technique makes it possible to extend the capability of measuring ozone to instruments not originally designed for that purpose. TOC retrievals over Antarctica using Sentinel-3/OLCI and MSI observations at various spatial resolutions (0.5x0.5 and 1x1 degree resolution)

Atmos 2021 – Conference Report and User Recommendations



4.11 Greenhouse Gases

Atmospheric carbon dioxide ((C_2)) and methane ((C_4)) measurements provide valuable information about sources and sinks of greenhouse gases (GHGs). Thanks to the new generation of space-based sensors, like the Japan's Greenhouse gases Observing SATellite (GOSAT) and GOSAT-2, the NASA Orbiting Carbon Observatory-2 (OCO-2) and OCO-3 missions, and the Copernicus Sentinel-5P, spatially resolved estimates of CO₂ and CH₄ columns with a global coverage are now available. In a keynote address, NASA-JPL showed how these new products can be used in inverse modelling to constrain top-down budgets and can complement national emission inventories leading to a better understanding of GHG exchanges between surface and atmosphere from biogenic as well as anthropogenic processes. The importance of fostering the collaboration of bottom-up and top-down modelling communities was stressed in order to define the best products and the best practices for combining those measurements. University of Bremen presented the Fast atmOspheric traCe gAs retrieval (FOCAL) algorithm, originally developed for OCO-2 retrievals with the focus on the derivation of XCO₂. FOCAL is a candidate algorithm for the upcoming CO2M mission. The new v3.0 of GOSAT/GOSAT-2 FOCAL is available with additional products to XCO₂ such as XCH₄, XH₂O, HDO (delta D)





and XN₂O. Validation with the TCCON network showed good results. It was clarified that the a-priori CO₂ vertical profiles are based on the novel SLIM model which is based on Carbon Tracker data in combination with growth rates. Regarding the N2O, the observed equator to poles gradient can be related to the effect of different tropopause heights.

SRON presented a convolutional neural network (NN) trained algorithm based on TROPOMI observations in combination with high-resolution instruments such as GHGSat, PRISMA, and Sentinel-2 to detect CH_4 emission sources. The synergy between medium and high resolution sensors work for different source types like landfills, coal mining and oil/gas extraction industry. The NN approach is also able to detect plumes with larger spatial extent like the emissions from wetland areas but with less precision than the single point sources.

Another approach to quantify local anthropogenic CH4 emissions has been developed by the University of Bremen based on the Weighting Function Modified Differential Optical Absorption Spectroscopy (WFM-DOAS) algorithm and applied to TROPOMI data. The algorithm is able to detect emissions from productive oil, gas and coal basins based on daily observations. The main uncertainty in the emission estimates is caused by uncertainty in the wind speed.

The rapid increase in air temperature over Northern latitudes is impacting the cryosphere with increasing human activity also being responsible for higher levels of methane emissions. The column-averaged methane (XCH4) observations from TROPOMI provides unprecedented coverage in this region, compared to previous satellite missions or in-situ measurements. FMI presented a systematic comparison of three TROPOMI methane products: operational and scientific SRON products, and the scientific WFMD product. The study focused exclusively on latitudes poleward of 50°N and evaluated the XCH₄ biases at four high-latitude TCCON sites. The polar vortex equally affected the performances of both TROPOMI and TCCON stations, and



Detection of a methane hot-spot over a gas pipeline in Kazakistan by combining the Copernicus Sentinel-5P and Sentinel-2 missions.





the differences between the satellite's products were larger than the TCCON comparison suggested. FMI assessed that also infra-red sounders can be a powerful source of data at these latitudes in all seasons, but they are characterised by a limited sensitivity to the surface and therefore to the local fluxes.

In the framework of the ESA Methane+ project, SRON presented a synergistic methane retrieval between SWIR and TIR bands using TROPOMI and IASI data. Global model inversions have been performed with this dataset from spring 2018 to early 2020 showing a rapid increase in global CH4 during the Covid-19 pandemic. This is also reported from the global surface measurements network and further studies on 2019-2020 growth rate change needs to account for the possible impact of changes in OH.

The capabilities of WorldView-3 (WV-3) for mapping methane point source emissions at high spatial resolution (3.7 m²) have been shown by Universitat Politecnica de Valencia (UPV). The proposed retrieval methodology is based on a multiple linear regression of six SWIR bands barely affected by methane absorption against the B7 (2235-2285 nm) that is positioned at a highly-sensitive methane absorption region. The potential of WV-3 for methane mapping has been further tested under real-case studies with a positive detection of 26 different point source emissions covering different methane hotspot regions with the capability to detect small leaks. UPV concluded that the plumes have been quite easy to detect in homogeneous surfaces. Data from WV-3 are in general provided after two months from the request.

The combination of TROPOMI regional scale data with high spatial resolution from hyperspectral and multispectral satellite instruments such as PRISMA and Sentinel-2 creates an ideal framework for the detection and the quantification of methane emissions point sources. With this synergistic approach UPV detected 29 point emitters in Turkmenistan and demonstrated that. Using Landsat 4 and 5, it is possible to detect emission sources that were already active in the 1980's. Methane detection is feasible with Landsat 4-5-7 and 8, possibly also Landsat-9. Further studies are needed in order to compare methane retrievals from the different Landsat platforms.



FMI presented a new methodology for deriving source-specific emission ratios of nitrogen oxides (NOx) to carbon dioxide (CO₂) by means of TROPOMI and OCO-2 observations. The approach is based on scaling the observed ratio along the OCO-2 track with simulated data, in order to obtain the NOx-to-CO₂ emission ratio at the source. The approach has been tested for the Matimba power station in South Africa showing a good agreement with existing inventories. It has been specified that for the emission estimates the wind speed is implicitly included in the model simulations, so there is a dependence on the wind speed but it is not a multiplicative factor and they don't have to determine what is the effective wind speed. The main uncertainties in this approach are related to NOx lifetime.

The impact of scattering related XCO₂ uncertainties in CO₂M data on inferring CO₂ fluxes from cities has been investigated by SRON. Synthetic CO₂M data were perturbed according to XCO₂ uncertainty characteristics derived with a neural network approach. Results showed more accurate estimates for China cities with respect to European cities and this can be explained by larger XCO₂ enhancements due to higher emissions in China.

High latitudes pose significant challenges to reliable space-based observations of total column carbon dioxide (XCO₂) because snow-covered surfaces absorb strongly in the near-infrared wavelengths coinciding with the CO₂ absorption channels of the Copernicus Anthropogenic CO₂ Monitoring (CO₂M) Mission. FMI presented a feasibility study of CO₂ retrievals over snow from simulated CO₂M radiances. The team evaluated results against the ground-based XCO₂ retrievals from the Total Carbon Column Observing Network (TCCON), and identified the snow-covered satellite pixels using auxiliary snow coverage data. The full CO₂ swaths were simulated over snow and only small changes in the TOA radiances have been observed. The TOA radiance decrease was observed simulating off-glint angles of 1, 3 and 6 degrees.

The CO2M satellite mission will provide new capabilities of imaging CO₂ and NO₂ which enables a quantitative assessment of CO₂ emissions at the scale of large point sources such as power plants. The CO₂













signal may be compromised by biospheric signals, and may be obscured by cloud cover. EMPA presented first results for the application of computer vision techniques to enhance and detect plumes in CO₂ and NO₂ images The first technique is 'denoising', to suppress incoherent additive (not just Gaussian) noise in the CO₂ and NO₂ images. The second technique is 'inpainting', to perform missing data interpolation due to cloud cover using a U-net style convolutional neural network. The third technique is 'ridge detection', to identify plumes based on their structural properties rather than just their enhancement over the background. It has been clarified that inpainting technique should be applied with cloud cover less than 10% and anomaly amplitudes of the plumes are well reproduced by the method that has been tested also for turbulent plumes.

DLR presented the satellite mission concept "CO₂image" that will complement the suite of planned CO₂ sensor able to detect small point sources with a spatial resolution of 50x50 m2. A fleet of CO2Image 4.12 Aerosols sensors would be able to monitor roughly 80% of the CO₂ emissions from coal-fired power plants worldwide. One mission design element relates to adjusting local overpass times in order to achieve DLR presented an ensemble algorithm for AOD applied within the Copernicus Climate Change Service the mission objectives considering the diurnal variability of turbulence, cloud cover, wind speed and (C3S) to several sensors: AATSR (and ATSR-2), SLSTR, OLCI and IASI. This algorithm uses the pixeluncertainty, and measurement geometry. First results suggest an advantage to measuring earlier in level uncertainties of several algorithms for the same sensor. Before calculating the ensemble results, the day, in contrast to the afternoon overpass time of most current missions targeting greenhouse the pixel-level uncertainties of all algorithms/instruments were evaluated against true errors versus gases. The instrument will be able also to retrieve methane. DLR also clarified that it is important to AERONET. Validation of gridded daily ensemble products showed clear beneficial effects for the IASI look closely at the boundary layer evolution relevant for measurements and models especially in early ensemble, slight effects for ATSR-2 and SLSTR and limited impact for OLCI. morning conditions.

In the 2020s a number of satellites with Multi-Angle Polarimetric (MAP) instruments will be launched. Total column concentrations of GHGs and other climate relevant gases retrieved from ground-based KNMI showed the great potential of these polarisation sensitive sensors to retrieve high quality information solar absorption measurements using Fourier transform infrared (FTIR) spectrometers used in the Total on aerosol optical properties (size distribution, refractive index, shape). In the framework of the HARPOL Carbon Column Observing Network (TCCON) are a primary source of reference data for validating satellite project two full inversion algorithms (GRASP and RemoTAP) have been presented identifying for each data. Instruments sample the whole atmospheric column, similar to the satellites. BIRA-IASB presented of them strong/weak points and suggesting the optimized approach to retrieve aerosol properties. As portable low-resolution FTIRs, one of which is the EM27/SUN that is used by the Collaborative Carbon it was noted, the objective of the HAPROL project is to suggest the potential optimizations of aerosol

Column Observing Network (COCCON). These low resolution spectrometers allow a denser distribution of the ground-based stations providing high quality data comparable to TCCON stations. Data from these instruments is already available for the satellites products validation activities.

In the Sentinel-5P +Innovation TROPOSIF project, Universitat Politecnica de Valencia presented a global dataset of Solar Induced Fluorescence (SIF) from TROPOMI observations. The TROPOSIF dataset covers the period from May 2018 and August 2021 including SIF retrievals from two different fitting windows. Also surface reflectance in seven spectral positions are included in the datasets as an ancillary variable to be used in combination with SIF. SIF data are closely related to the plant photosynthesis activity. The new dataset has the aim to foster studies on Gross Primary Production (GPP) that will be a product from future Sentinel missions.

scattering modelling as well as the land surface and ocean reflection models to be used in MAP retrievals.

Since aerosols affect climate in several ways, DLR presented regional trends of AOD from Dual-View instruments (ATSR2, AATSR, SLSTR and IASI). Trends have been calculated using a seasonal Mann-Kendall-trend-test after a bias correction between the different instruments and then compared to AERONET ground-based observations. Results revealed that trends of different algorithms using dual view instruments are mostly consistent while for IASI are partly consistent.

Times series of AOD over China for the years 2000-2021 using TROPOMI and OMI observations have been presented by KNMI. Despite large spatio-temporal fluctuations with differences between provinces, results showed that AOD over south-eastern China has stabilised in recent years at a value similar to the AOD in 2020 thanks to the implementations of a series of clean air action plans.

Stratospheric aerosols play a crucial role in the Earth system and in the climate. The strong coupling between the stratospheric aerosols and stratospheric ozone amounts determines the need of global long term aerosols records for climate modelling studies. University of Bremen presented the Global Space-based Stratospheric Aerosol Climatology (GloSSAC) comprising merged data of extinction coefficients from 10 instruments covering the period from 1978 to 2018. The team found a good agreement between the long time series from SCIAMACHY, OMPS and OSIRIS without identifying drifts and noticed that volcanic features are seen by all instruments.

In the framework of the ESA Sentinel-5P +Innovation AOD/BRDF project, GRASP and KNMI



19 June 2020.





presented an innovative framework for aerosol and surface retrievals from TROPOMI. It integrates the data and Sentinel-4 synthetic data have been provided. In the latest algorithm versions, the surface advanced Generalised Retrieval of Aerosol and Surface Properties (GRASP) algorithm and the heritage albedo climatology has been replaced with TROPOMI daily albedo retrievals (GE_LER) and a detection AOD and directional Lambertian equivalent reflectivity (DLER) algorithms. Results from validation of AOD flag is added to identify ice clouds. It was clarified that the ice flagging uses a simple threshold approach and aerosol properties showed a very good agreement with AERONET surface observations and a fair using CRB height and temperature profile from ECMWF. agreement at global scale with well-validated aerosol and surface products from MODIS and VIIRS.

Arctic amplification describes the recent period in which temperatures are rising twice as fast as the More insight into the Sentinel-5P +Innovation AOD/BRDF DLER algorithm has been provided by KNMI global average producing effects on Artic's reflectivity that is dependent on the ice shelf and to the showing substantial improvements on the surface characterization evaluated by using TROPOMI geometry presence of clouds. DLR presented an investigation of the changes in the spectral reflectance at the top observation. The new LER products were integrated as ancillary information in the GRASP algorithm of the atmosphere (Rtoa) at different wavelengths by means of GOME and SCIAMACHY observations. This info is coupled with cloud properties and fluxes at the top of the atmosphere and shows distinct areas providing state-of-art aerosols and surface characterization including Angstrom exponent, single scattering where the reflectivity diverges. While darkening areas can be attributed to seasonal sea ice decline, an albedo and surface BRDF and DLER. increase of Arctic brightness over sea ice free regions can be attributed to changes in the clouds optical properties. DLR stressed the importance of supercooled clouds in the Arctic as already proved by in-situ Several studies have shown that aerosol retrievals are strongly affected by cloud contamination especially

in the transition zone between cloud and cloud-free pixels. The choice of the cloud mask is thus a critical point. Rayference presented the new version of the CISAR algorithm applied to SLSTR observations. Aerosols are retrieved in the vicinity of clouds as well as within optically thin clouds, assuring a larger spatial coverage than traditional aerosol retrieval algorithms. The validation against AERONET showed a good temporal evolution agreement while the global comparison with MODIS showed good spatial distribution and no systematic bias.

4.13 Clouds

DLR presented its operational cloud retrieval algorithms called Optical Cloud Recognition Algorithm (OCRA) and Retrieval of Cloud Information using Neural Networks (ROCINN). The ongoing Sentinel-5P and the future Sentinel-4 missions focus on atmospheric composition covering the UV/Vis/NIR spectral range allowing the retrieval of basic cloud information. An application of both algorithms for real Sentinel-5P

Atmos 2021 – Conference Report and User Recommendations



campaigns and assessed that polarisation measurements could be very useful in distinguishing between different cloud types and surfaces.

Three-dimensional cloud structures may impact atmospheric trace gas products from UV/Vis sounders. NILU presented a study based on synthetic data and observational data to identify and quantify the possible cloud-related bias in NO₂ tropospheric vertical column retrievals. Two synthetic set-ups are considered: the first include simple 2-D clouds with various geometrical and optical thicknesses and the second with a realistic 3-D information from ICON large eddies simulation. It has been shown that cloud shadow has important effects on NO₂ polluted profiles with bias around 10% for low zenith angles that increase for larger SZA.

Using global satellite-based cloud and radiation datasets and global sea ice and sea surface temperature datasets University of Melbourne presented an analysis on trend variability of cloud and radiation properties





over the Southern Ocean and their links to Antarctic sea ice. The team found an increased fraction of high clouds at higher latitudes coincides with increasing precipitation. During the sea ice growth season sea ice concentration (SIC) anomalies are negatively correlated with net radiation flux anomalies, but correlation with cloud cover is much weaker. While during the ice melting season SIC anomalies are negatively correlated with total cloud cover, but correlation with net radiation flux is less evident. It has been clarified that these findings are related to the Arctic (e.g. Atlantic Ocean) while the Antarctic continent may have a different behaviour.

Cloud shadows observed by TROPOMI can contaminate air quality products because they are generally not taken into account in the models used for the retrievals. KNMI presented the Detection AlgoRithm for CLOud Shadows (DARCLOS) for TROPOMI. KNMI states that this is the first cloud shadow detection algorithm for spectrometer instruments. DARCLOS has been validated with true colour images from VIIRS instruments and demonstrated that potential cloud shadow flag (PCSF) can be used to exclude any cloud shadow contamination from TROPOMI Level 2 data.

4.14 Water Vapour

Atmospheric moisture is a key factor for the redistribution of heat in the atmosphere, and there is a strong coupling between atmospheric circulation and moisture pathways which is responsible for most climate feedback mechanisms. Water vapour isotopologues can make a unique contribution to a better understanding of this coupling. University of Leicester developed a new retrieval of water vapour isotopologues for TROPOMI, specifically of the ratio of HDO/H2O, based on their Full Physics (UoL-FP) retrieval algorithm. Retrieval performances have been validated against ground-based observations from MUSICA NDAAC and TCCON networks and also intercomparisons with IASI and GOSAT satellite data have been carried out.



Daily cloud fraction computed from TROPOMI observations on board Sentinel-5P.







SRON presented updates on an HDO/H_2O column data retrieval from TROPOMI including clear-sky and cloudy scenes. Including scenes with low clouds there is a large enhancement in data coverage especially over oceans. Data was validated against TCCON observations with a very good agreement. Bias corrections have been performed both for H_2O and HDO. It was assessed that a homogenization between TCCON and MUSICA datasets is fundamental for the validation of water vapour observations from satellites.

DLR showed results from the retrieval of total column water vapour (TCWV) from TROPOMI in the visible blue spectral band (435-455 nm) using the GE_LER albedo derived from TROPOMI. The TROPOMI TCWV algorithm follows the typical two step approach with spectral fit retrievals of slant columns and conversion to vertical columns using iterative AMFs. Cloud parameters are taken from the operational TROPOMI cloud product developed by DLR. The results are validated by comparing ERA5 reanalysis data, GOME-2, MODIS and Special Sensor Microwave Imager Sounder (SSMIS) satellite observations showing a very good agreement. MPI presented the retrievals of TCWV from OMI in the spectral band (430-450 nm) based on the DOAS approach. In order to investigate changes in TCWV, multiple years of OMI observations (2005-2020) were presented showing significant positive trends. Similar trend patterns were found also from ERA5 and ESA GOME-Evolution datasets. ERA5 data used for the validation showed more reliable results over ocean than over land.

University of Leicester investigated the residence time of water vapour in the atmosphere, between evaporation and precipitation, from satellite observations, reanalysis and model ensembles. Turnover times (TUT) from models showed differences between 2.5 and 7.5 hours relative to satellite observations with a greater complexity at regional scales. In general the model trends for TUT showed a general slowing of the hydrological cycle which is not observed both in reanalysis records and satellites. The importance of relating the TUT

Atmos 2021 – Conference Report and User Recommendations



Atmospheric moisture is a key factor for the redistribution of heat in the atmosphere and there is strong coupling between atmospheric circulation and moisture pathways which is responsible for most climate feedback mechanisms. TROPOMI water isotopologues observations can make a unique contribution for better understanding this coupling.







rate changes with respect to surface temperature has been discussed. The available time series may not for tropical eruptions at tropopause level and an underestimation for ash-laden plumes. The presence of be long enough to make assumptions on a climate trend though. ice in volcanic clouds, which characterised e.g the Etna 2021 eruptions, is not taken into account in the algorithm. However, in the UV region ice clouds are absorbing only at low levels.

BIRSA-IASB presented vertically resolved water vapour climate data records (CDR) recently released by ESA's Water Vapour Climate Change Initiative (CCI) project. Merging strategies and the general Usually, horizontal homogenous atmospheric properties are assumed for the analysis of satellite characteristics of these CCI data records have been presented and related to other CDRs developed by observations of atmospheric trace gases causing only small errors in the retrievals. For volcanic plume NASA and NOAA. Multiple linear regression was applied to all time series to infer the seasonal cycle and retrieval this assumption leads to large errors. The Max Planck Institute for Chemistry (MPIC) investigated a related disagreement has been discussed. It was underlined that not only the water millennium drop with the 3D Monte-Carlo radiative transfer model TRACY-2 three different 3D effects: a) geometric light path effects: the light path from the sun to the surface and that from the surface to the satellite might can be observed from all time-series but also another drop in 2014 needs to be further investigated. not both cross the volcanic plume; b) effects of horizontal light paths: light scattered into the FOV might originate from regions outside the volcanic plume and thus lead to a decrease of the absorption signal; 4.15 Volcanic Emissions c) saturation effects: for narrow plumes the SO₂ absorption signal can be strongly suppressed since most of the backscattered light is absorbed by SO₂ itself.

Determining the height of SO₂ clouds after volcanic eruptions is a challenging task in UV satellite retrievals but it can be considered as the most important parameter to forecast the motion, velocity, and transport of a volcanic cloud. With that it is an essential parameter for local authorities and aviation safety decision makers. In the framework of the Sentinel-5P +Innovation project, DLR developed a combined principle component analysis and neural network retrieval algorithm called 'Full-Physics Inverse Learning Machine' (FP_ILM), which enables extremely fast (3 ms per TROPOMI pixel) yet accurate (<2 km accuracy) SO₂ LH retrievals for SO₂ columns higher than 20 DU. The SO₂ layer height product has been validated successfully against IASI, OMI and CALIPSO observation and is actively assimilated by ECMWF/CAMS.

There are still numerous volcanoes that are well characterised using ground measurements and direct observations, known to be passively degassing, and that are still below the detection limit for satellite BIRA-IASB presented the Covariance-Based Retrieval Algorithm (COBRA), a new SO₂ LH algorithm based observations. University of Manchester presented long-term averaging of TROPOMI observations of on TROPOMI observations that relies on an iterative approach making use of SO₂ optical depth look-up-SO₂ columns retrieved with the COBRA algorithm. The Soufrière Hills volcano has been monitored using tables. The major improvement of this algorithm relates to the sensitivity of the SO₂ LH product from 20 DOAS network data, while the plume is not visible from daily satellite imagery. Statistically, the west DU to 5 DU. Comparisons have been carried out with CALIOP, MLS and IASI observations for a number wind direction was prominent for 85-90% of the year. This is advantageous in the sense that gas will of volcanic eruptions showing an overall good agreement. However, a slight overestimation is observed

Atmos 2021 – Conference Report and User Recommendations

Bromine monoxide (BrO) can influence atmospheric chemical processes due to the ozone abundance in the polar boundary layer, in the stratosphere and in volcanic plumes. MPIC provided a global overview of BrO/SO₂ molar ratio using TROPOMI observations following a DOAS algorithm approach. Calculated BrO/SO₂ ratios differ strongly between different volcanoes, variability for the same volcano is found at different points in time ranging from 10-5 up to several 10-4.











be blown in the same direction for most of the year, making the averaging technique more effective and making SO₂ plume visible also for TROPOMI. Before averaging a detailed SO₂ background was computed.

BIRA-IASB presented the ALARM (multi-hAzard monitoring and earLy wARning systeM) project aiming at developing a global multi-hazard monitoring for aviation safety in case of natural phenomena, severe weather or aerosol/gas episodes from natural hazard. The system uses satellite observations, ground-based network data and model forecasts to provide three different levels of information to stakeholders. First the early warning with the hazard geolocation and the level of severity, second the nowcasting and forecasting for the hazard evolution at the flight level. The actual ash amount is also retrieved directly and not estimated from the SO₂ amount.

4.16 OCIO, BrO, Glyoxal

The University of Bremen presented a novel algorithm for the retrieval of chlorine dioxide (OCIO) from TROPOMI, developed in the framework of the Sentinel-5P +Innovation project. While OCIO is not directly involved in stratospheric ozone depletion, it can serve as a quantitative indicator for stratospheric chlorine activation. The OCIO product from TROPOMI showed an excellent signal to noise ratio, small offsets and low scatter compared to data from previous sensors. Chlorine activation is observed in both hemispheres, with strong variability in the Northern hemisphere during the period 2018-2021 while in the Southern hemisphere there was less variation but with differences between the different years. The product has been validated against ground-based observations with excellent agreement. Also visible in the OCIO data is a discontinuity originating from a new TROPOMI Level 1 dataset.





The MPIC presented a comparison between column densities of OCIO from TROPOMI observations with meteorological data and CALIPSO Cloud-Aerosol LIDAR with Orthogonal Polarisation (CALIOP) polar stratospheric cloud (PSC) observations for both Antarctic and Arctic regions. OCIO SCDs also coincide well with CALIOP measurements for which PSCs are detected. Very high OCIO levels are observed for the Northern hemispheric winter 2019/2020 with an extraordinarily long lasting and stable polar vortex being even close to the values found for Southern Hemispheric winters. Main differences between the University of Bremen and MPIC OCIO retrievals relate to differences in selected fitting windows and the approach on correction terms. Here MPIC uses a physics based methodology while University of Bremen applied empirical corrections.

First observations of stratospheric bromine nitrate (BrONO2) derived from MIPAS have been presented by KIT. Simulations with the EMAC (ECHAM/MESSy Atmospheric Chemistry) model of stratospheric BrONO₂ have been conducted and showed a model underestimation of enhanced BrONO₂ in the polar winter stratosphere above about 30 km, a higher modelled values than observed globally in the lower stratosphere (up to 25 km) most obvious during night, and lower modelled concentrations at low latitudes between 27 and 32 km during sunlit conditions. Cloud parameterization and air mass factor in EMAC have been obtained from the model itself, no data have been used.

Since halogen radicals can drastically alter the atmospheric chemistry in the Polar regions, MPIC showed how TROPOMI observations allow the detection of the mechanism that regulates the release of bromine compounds, called the bromine explosion. Tropospheric columns of BrO are retrieved from TROPOMI with a DOAS algorithm and the separation between tropospheric and stratospheric columns is obtained relying on NO₂ and O₃ observation from the same instrument. Events of bromine explosions have been found for spring 2019 and 2020.



Chlorine activation over Antarctica seen by TROPOMI on board Sentinel-5P in September 2021.





Glyoxal (CHOCHO) in the atmosphere originates from the oxidation of biogenic and anthropogenic nonmethane volatile organic compounds (NMVOCs). CHOCHO observations are therefore useful to provide information on global NMVOCs emissions. In the framework of the Sentinel-5P +Innovation project BIRA-IASB developed a DOAS algorithm able to retrieve CHOCHO columns densities from TROPOMI. The algorithm has been extended also to other satellite nadir sensors such as OMI, GOME-2A and 2-B in order to temporally expand the CHOCHO time series. Comparison with ground-based MAX-DOAS glyoxal measurements has been carried out showing a good agreement. Satellite and ground-based instruments capture similar CHOCHO variability while showing a low bias during winter for mid/high latitudes.







5. e-Posters/Lightning Talks Sessions Summary & Highlights

5.1 Air Quality

DLR presented a study on the relation between economic development and air quality over the Po Va looking primarily at NO₂ concentrations by means of ERS-2, Envisat, MetOp-A and MetOp-B observatio First significant relations, with fewer NO₂ pollution outbreaks, were found in 2008 caused by the glo financial crisis followed by a second correlation between 2009 and 2014.

UFS GmbH described the activities of the Virtual Alpine Observatory (VAO), a network of 12 high altit research stations deployed throughout the Alpine region. VAO aims to contribute to a better understand of environmental processes in the Alpine region. Outcomes and results of the work will support decise makers by balancing economic, social and environmental interests in a sustainable way.

Academy for Mathematics, Science, and Engineering presented a review on machine learning algorith tailored for air quality. The team provided a unified and systematic survey of the current machine learn algorithms used to solve multiple air quality monitoring tasks.

University of Punjab showed an assessment of the air quality over Pakistan by using Sentinel observations. Maximum concentrations of CO, HCHO and SO, were found during summer, winter and monsoon season, respectively. The concentration of SO_2 increases to about 135.7% and 165.6% of Quetta and Peshawar.

FMI estimated ground level NO₂ concentrations over Finland from TROPOMI using methods by Lam et al. (2008) and Cooper et al. (2020) based on the GEOS-Chem chemical transport model. FMI found

illey ons. obal	that the method by Cooper et al. (2020), which includes a correction for the vertical distribution of NO ₂ within the boundary layer, overall performs better than the method by Lamsal et al. (2008) with no such correction.
ude	DLR presented the AlpAirEO project in the framework of ESA's EO4Alps initiative. AlpAirEO will provide timely information on the aggregated health risk by air pollution and thermal stress covering the Alpine area. Preliminary analyses show that the population weighted health burden for main cities exhibits no
ding sion	clear trend albeit intensifying efforts and control measures by EU and local authorities.
mc	To realise the full potential on air quality assessment of future constellations of LEO (e.g. Sentinel-5P) and GEO (e.g. Sentinel-4) satellites BIRA-IASB presented the major issues that must be addressed. The sub-city scales and the resolution of satellite data must be enhanced and also the non-trivial relation
ning	between satellite and surface concentrations need further studies.
-5P pre- over	University of Rotterdam combined the high-density air pollution network of the citizen science initiative Hollandse Luchten around Amsterdam with remote-sensing data to form observation clusters of air pollution concentration. The team also presented open and freely accessible methods, procedures and data used to develop urban air pollution forecast prototypes.
nsal d	University of Thessaloniki used Sentinel-5P/TROPOMI NO ₂ observations in order to estimate updated NOx emissions over four of the largest power plants in NW Greece. LOTOS-EUROS chemical model simulations were used in order to find the best matching emissions to the Sentinel-5P/TROPOMI observations





5. e-Posters/Lightning Talks Sessions Summary & Highlights through a data assimilation technique. The findings were validated by comparing NO₂ surface simulations pollution and detect new hotspots in South Asia during July 2018 to September 2021 by University of from both free and assimilated CTM model runs to NO₂ in-situ measurements from an air quality station Punjab. Also, a comparison of spatial distributions of NO₂ retrieved from TROPOMI and OMI has been near the largest power plant.

The lockdown in Pakistan due to the Covid-19 pandemic has reduced air pollution in mega-cities (Lahore, Karachi, Islamabad and Peshawar) during March, April and May 2020 as shown by University of Punjab. Satellite observations from Sentinel-5P over these cities indicate that NO₂ emissions dramatically reduced in March 2020 as compared to the same month of the previous year, with a maximum decrease of ~16% in Lahore. The related change of Aerosol Optical Depth (AOD) was found with a maximum decrease of ~52% in Lahore.

A new lane separation methodology for the maritime sector emissions attributed to different vessel types and marine traffic loads in the Mediterranean and the Black has been applied by University of Thessaloniki weeks before both measurements. using TROPOMI NO, data. TROPOMI can detect significant shipping lanes in the Mediterranean on both seasonal and annual temporal scales. The implementation of this new lane separation methodology is University of Oslo derived a spatially continuous surface NO₂ ¬oncentration from tree-based machine learning models such as Random Forest and Extreme Gradient Boosting (XGBoost), using datasets able to differentiate the NO₂ originating from diverse shipping activities. The cargo vessels are the highest emitting sector in the Mediterranean and the Black Sea regions followed by fishing, tanker, passenger, such as tropospheric NO₂ from TROPOMI, day-night band from the Visible Infrared Imaging Radiometer Suite (VIIRS) instrument, NO₂ station measurements from the European Environmental Agency (EEA) and other vessels. and secondary variables such as meteorological parameters and land use land cover information. The BIRA-IASB investigated the NO₂ distribution in Flanders as recorded by ground-based concentration preliminary outputs of this work show promising results with a mean absolute error of 10.4 μ/m^3 measurements, airborne data and remotely-sensed density columns, with the help of the high-resolution and 12 μ/m^3 respectively for Random Forest and XGBoost models.

WRF-Chem chemical-transport model as a cross-comparison tool. Simulated NO₂ distributions are hyperspectral imager APEX and spaceborne NO₂ columns obtained by TROPOMI.

compared against values from monitoring stations in Flanders, vertical columns measured by an airborne FMI used the data to support air quality assessment in two different ways. First a long-term average over Finland was calculated in order to find the average CO distribution and to recognize areas with possible larger sources. Further, satellite observations in combination with ground level data from scientific monitoring stations in Helsinki, Sodankylä and Pallas were used to estimate ground level CO Tropospheric NO₂ retrievals (Level-2) from TROPOMI have been used to observe the current state of NO2

performed. Over strongly polluted areas, TROPOMI retrievals show ability to effectively detect new and small size hotspots, and to segregate nearby mega sources. In Afghanistan, Kabul city is more clearly appearing as a hotspot. In Pakistan, the newly installed Sahiwal coal-based power plant was undetectable by OMI retrievals.

Airborne measurements of biomass burning pollution trace gases in the upper troposphere from the Gimballed Limb Observer for Radiance Imaging of the Atmosphere (GLORIA) have been presented by Karlsruhe Institute of Technology. With the help of backward trajectories KIT showed that measured pollutants are likely originating from South America and central Africa. In the same regions, elevated peroxyacetyl nitrate (PAN) mixing ratios are visible at the surface layer of the CAMS model during the













concentrations by means of a simple linear relation between ground level concentrations and the total emission reductions during the Covid-19 lockdown in spring 2020 over Europe. CNRS found clear column concentrations provided by satellite measurements. enhancements of near-surface ozone in Central Europe and Northern Italy, and some other hotspots, which are typically characterised by VOC-limited chemical regimes. An overall reduction of ozone is Airborne in-situ measurements of sulphur dioxide (SO₂) emissions plumes from two coal-fired power observed elsewhere, where ozone chemistry is limited by the abundance of NOx. plants in Bosnia-Herzegovina (Tuzla) and Serbia (Nikola Tesla) were carried out with the German research aircraft Falcon-20 by DLR. Results were compared against TROPOMI measurements showing some A complete characterization of the TROPOMI tropospheric ozone, providing clues to properly include it in

problems with dense smoke clouds frequently covering these countries in winter. First estimates by means of a mass balance approach showed that the SO₂ mass flux from Tuzla is about twice as high as indicated by common emission inventories.

5.2 Ozone

University College London (UCL) conducted a study on the impact of rocket launches and space debris impact on stratospheric ozone. UCL added an inventory of pollutant emissions from rocket launches and re-entries of both reusable spacecraft and debris during 2019, to the 3D global chemical transport model GEOS-Chem finding that chlorine, emitted by solid rocket motors, is the most deleterious to stratospheric ozone, in agreement with previous studies.

Vertical ozone profiles retrieved from the special viewing mode of Brewer and Dobson spectrophotometers called Umkehr were discussed and compared against NASA SBUV v8.6 by University of Thessaloniki finding a good agreement. These ozone profiles can be used for the validation of both satellite IR instrumentation, that cover from the UTLS upwards, as well as UV instrumentation, that also cover the troposphere albeit with a coarser vertical resolution.

Surface ozone concentration in ambient air is influenced by background value, regional and local chemical CNRS presented a comprehensive study integrating satellite observations of ozone pollution in-situ generation, deposition, chemical removal and interregional transport comprehensively, and then a formula for the calculation of surface ozone concentration is formed. The University of Mining and Technology measurements and chemistry transport model simulations for quantifying the role of anthropogenic

the GOME-type tropospheric ozone Climate Data Records, was presented by BIRA-IASB. Despite a little TROPOMI bias (<2 DU) which varies somewhat with reference instruments and signs of a weak latitudinal pattern and a moderate seasonal pattern was found. TROPOMI data meets the needs of the atmospheric research community capturing the seasonal cycle, biomass burning episodes and intraseasonal variability.

In the framework of the Ozone_cci+ project nadir ozone profiles from different satellites instruments have been retrieved, improved and homogenised. To verify the fitness-for-purpose, BIRA-IASB applied to ozone profiles products the versatile QA/validation system Multi-TASTE, which has been developed in the context of several heritage projects of ESA, EUMETSAT, and the European Commission.

A typical ALTIUS satellite mission orbit consists of the following measurement sequence: sunrise occultation, limb scattering observations in the dayside, sunset occultation and, in the nightside, stellar, planetary and lunar occultations. The sequence of stars, moon and planets that will be observed during each night-part of the orbit should be planned to ensure the best spatial coverage and to minimise the time it takes for the satellite to turn to a new target. BIRA-IASB presented the Dijksta's algorithm, one of the candidates algorithm to solve this problem.













presented the Light Gradient Boosting Machine (LGBM) algorithm able to integrate various satellite-based variables, numerical model-based meteorological variables and land variables in the above calculation formula to obtain the high spatial resolution surface concentration of ozone in China.

In the framework of the Tropospheric Ozone Assessment Report (TOAR), BIRA-IASB reported on the vertical harmonisation of tropospheric ozone time series recorded by past and present satellites. First results were illustrated with tropospheric ozone data records from GOME-2, IASI, OMI and TROPOMI, based on two approaches: (1) a model is used to match prior profile (and prior constraint) information in given retrievals; (2) a method is applied that removes a priori information from atmospheric state profiles that are obtained through an optimal estimation retrieval.

A comprehensive analysis of the temporal stability of stratospheric ozone profile data records by seventeen limb and occultation satellite sensors and by the ground-based instruments, ozonesondes, stratospheric LIDAR and microwave radiometer monitoring networks (NDACC, WMO GAW, SHADOZ) has been carried out by BIRA-IASB. Estimates of the stability of single profile data by limb/occultation sensors (Level-2) with respect to the ground-based networks were presented.

In order to detect regional trends of stratospheric ozone FMI presented MErged GRIdded Dataset of Ozone Profiles (MEGRIDOP) in the stratosphere with a resolved longitudinal structure, which is derived from data by six limb and occultation satellite instruments: GOMOS, SCIAMACHY and MIPAS on Envisat, OSIRIS on Odin, OMPS on Suomi-NPP, and MLS on Aura. Zonal asymmetry/structures in the climatological ozone profiles at middle and high latitudes associated with the polar vortex was found. At Northern high latitudes, the amplitude of the seasonal cycle also has a longitudinal dependence.

Several atmospheric CO₂ products, such as ACOS, NIES, OCFP and SRFP products from the full physics retrieval algorithm, provide CO₂ surface flux of GOSAT. In order to obtain the CO₂ data set with high precision, low uncertainty and high coverage, University of Mining and Technology used the products Tropical tropospheric columns ozone were retrieved by University of Bremen using TROPOMI observations

with the convective cloud differential (CCD) method Cloud Height adjusted Ozone Reference Algorithm (CHORA), while upper tropospheric ozone volume mixing ratios by means of the cloud slicing method CHOVA (Cloud Height induced Ozone Variation Analysis). The retrieval results are used to calculate monthly mean volume mixing ratios in the Pacific sector to height adjust the CHORA above cloud column ozone (ACCO) to a fixed pressure level.

5.3 Greenhouse Gases

The multiband instruments on board Sentinel-2 and Landsat satellites can detect methane emissions from super-emitters as the resulting methane column enhancement at a spatial scale of 20 to 30 m near the source produces sufficient absorption signal integrated within the broader short-wave infrared bands. SRON presented a machine learning-based methane leak monitoring system that uses convolutional neural networks (CNN) to automatically detect methane plumes using Sentinel-2 data at numerous point sources across the globe.

A new retrieval methodology for methane uses the SWIR band (2100-2300 nm) of Sentinel-2, which is sensitive to methane absorption. In order to calculate methane transmittance, the band 12 spectral channel is normalised by a 'methane-free' reference band, which can be estimated by means of different methodologies such as band regression and/or temporal normalisation. Universitat Politecnica de Valencia focused on the retrieval performance attending to factors such as the temporal misregistration, angular differences or spectral mismatch.









of the above four algorithms for fusion. Since the products of the same satellite are used, there is no covering absorption bands of CO₂ and CH₄ between ~1575 and ~1700 nm with a spectral resolution of need to consider the matching of time and space factors. The fusion results were encouraging, not ~1.1 nm. It is designed to detect and quantify CO_2 and CH_4 emissions from point sources, and serves as precursor and demonstrator for the larger 2-channel imaging spectrometer MAMAP2D, which is currently only increasing the coverage of XCO₂, but also demonstrating a good accuracy in validation with TCCON in the development phase. observations.

University of Bremen quantified the CO₂ emissions from localised sources such as power plants by using XCO₂ retrievals from the Orbiting Carbon Observatory 3 (OCO-3) in its snapshot area mode. They described a semi-automatic procedure to select promising targets and overpasses, a plume detection method using NO2 as a tracer for recently emitted CO₂ and an inversion technique to quantify CO₂ emissions from detected CO₂ plumes.

An algorithm to calculate CO₂ columnar abundance in tropospheric volcanic eruptions, based on a modified CIBR 'Continuum Interpolated Band Ratio' remote sensing technique plume, was presented by INGV. PRISMA (PRecursore IperSpettrale della Missione Applicativa) acquisitions, with a spatial resolution of 30 m, are used for the CO₂ retrieval and the algorithm has been tested over Stromboli and Etna volcanoes, both characterised by a persistent degassing phase.

University of Bremen presented a 3-year XCH4 dataset generated with the WFM-DOAS retrieval algorithm by using TROPOMI measurements with the aim to detect locally enhanced methane concentrations originating from emission sources. The algorithm identifies temporally stable local enhancements relative to the surroundings by defining a certain threshold that the local methane anomalies must exceed. To attribute the detected methane enhancements to potential sources the results are compared to inventories of anthropogenic methane emissions.

The MAMAP2D-Light instrument developed and built at the Institute of Environmental Physics at the University of Bremen for aircraft observations is a lightweight (~42 kg) single channel imaging spectrometer



5.4 Aerosols & Surface

DLR presented a novel aerosol retrieval algorithm using a radiative transfer model and the Tikhonov regularisation method to estimate aerosol layer height (ALH) and aerosol optical depth (AOD) from the TROPOMI 02A band (758-771 nm) measurements. The algorithm is optimised with a Bayesian-based aerosol model showing that in case of insufficient information for an appropriate micro-physical model selection, the optimised algorithm helps to find the most suitable aerosol model.

The National Observatory of Athens showed improvements of monitoring sea salt emissions where Aeolus wind profiles are assimilated in regional scale atmospheric models. Two different Weather Research and Forecasting (WRF) model configuration experiments were conducted, each one was initialised with different ECMWF IFS outputs; one with and one without assimilation of Aeolus Rayleigh and Mie L2B wind fields.

The GRASP algorithm was adapted for the combination of TROPOMI coarse (5.5 km by 3.5 km) and PRISMA fine (30 m) spatial resolution measurements. This combination allows transferring TROPOMI advantages of extended aerosol characterization to the high spatial resolution of PRISMA measurements. The results demonstrate a large potential of the approach based on the combination of instruments with coarse and high spatial resolution for aerosol sources identification and aerosol emission monitoring in high spatial resolution.









A first attempt to retrieve the AOD at 550 nm over land, using a deep neural network trained with optical and geometrical properties, during biomass burning events observed over Greece in the 2021 observations collected by MERIS, was conducted by DLR. The approach has three independent parts, summer fires. The measurements allowed the monitoring of the evolution of fresh smoke aerosols, as i.e. the preprocessor, the associator and the trainer, whereby the data are significantly reduced in size, well as to analyse its optical and geometrical properties (horizontal and vertical extent). matched spatio-temporally with data from the Aerosol Robotic Network (AERONET) and are finally trained with a neural network. Based on characteristics of high-frequency observations of the geostationary satellite Himawari 8, a new single scattering albedo (SSA) inversion algorithm using a radiative transfer model parameterized The Aerosol Index (AI) retrieved from TROPOMI's high spatial resolution observations presents specific by two-stream approximation was proposed by University of Mining and Technology. The team showed challenges as non-Lambertian cloud features, cloud shadows, and 3-D effects of clouds are now visible in results of SSA inversions over China and successfully validated against 7 AERONET sites for April 2020. the TROPOMI AER_AI data. An overview of plans to address these features in future AER_AI updates was given by KNMI, including also a description of the impacts on AER_AI due to the observed, wavelength-University of Leicester and the GRASP team from Lille retrieved aerosol properties from multi-angle polarimeter (MAP) measurements alone, and then used the retrieved aerosol properties as input for an dependent degradation in the TROPOMI irradiance and radiance data. XCO₂ retrieval only based on the high-resolution spectrometer for CO₂ measurements (CO2I) observations. The proposed approach uses the GRASP algorithm to infer aerosol properties from MAP measurements, In the framework of the ASKOS campaign for the validation of Aeolus products, one of the deployed instruments is EVE LIDAR a combined linear/circular polarisation LIDAR system with Raman capabilities and feeds its retrieved information to the UoL full physics CO, retrieval, which is based on optimal that retrieves the particle backscatter coefficient, the particle extinction coefficient, and the linear and estimation. circular depolarization ratios able reproduce the operation of the deployed LIDAR on board Aeolus. Targeted measurements of the EVE LIDAR system were performed by University of Thessaloniki every A first validation analysis of TROPOMI Aerosol Layer Height (ALH) has been conducted by INOE using independent, ground-based cloud-free observations taken at 18 sites in the frame of the European Aerosol Friday evening matching a close Aeolus overpass. Research LIDAR Network (EARLINET) during September 2017 - September 2021 and the Neural network Aerosol Typing Algorithm based on LIDAR data (NATALI). For overpass comparisons, ALH satellite pixels University of Bremen presented retrieval results of the geometrical extent of clouds based on near-infrared oxygen absorption from SCIAMACHY measurements. The team also showed a technique to inherently are averaged within 0.5 degrees radius around ground-based LIDAR location. account for aerosol perturbation of in-cloud extinction profiles based on the synergistic exploitation of

DLR presented a novel algorithm for the retrieval of geometry-dependent effective Lambertian equivalent oxygen absorption and multi-wavelength continuum in the solar spectral range.

reflectivity (GE_LER) from UVN sensors based on the full-physics inverse learning machine (FP_ILM) University of Thessaloniki analysed the impact of wildfires over Greece on atmospheric aerosol load retrieval. The GE_LER retrieval is optimised for the trace gas retrievals using the DOAS algorithm and the using satellite data. A synergy of satellite data from GOME-2 and TROPOMI is used to derive the aerosol large amount of data of the new atmospheric Sentinel satellite missions. The TROPOMI GE_LER/G3_LER













compared with climatological OMI and GOME-2 LER data.

data quality through successive version upgrades, using ground-based and satellite data. Cloud height data from three TROPOMI cloud products were compared to Radar/LIDAR based cloud profile information from the ground-based networks ACTRIS-CLOUDNET and ARM. A description of the latest development of the FRESCO for Sentinels (FRESCO-S) has been provided by KNMI. Regarding TROPOMI the main reasons for the changes are the high spectral resolution (narrower instrument spectral response function) and the variation of actual wavelength grid of TROPOMI. FRESCO-S products, retrieved from the O₂ A and B bands, include effective cloud fraction, cloud height (cloud pressure), scene albedo, and scene pressure. Breakthroughs in Radar technology have recently fostered the construction of two G-band (frequency between 110 and 300 GHz) ground-based systems: the NASA-JPL VIPR system and the UKSA/CEOI funded

results for the fitting windows corresponding to O₃, NO₂, SO₂, HCHO, H₂O, and clouds are presented and Cloud radiance data in the visible contain a wealth of information on clouds, but have never been assimilated in global numerical weather prediction models. ECMWF implemented the MFASIS (Method for FAst Satellite Image Synthesis) observation operator for monitoring cloudy reflectances allowing accurate simulation of cloud-affected visible satellite images, and is suited for operational applications in ECMWF's Integrated Forecasting System. Earth surface patterns are spatially very heterogeneous and available ground-based measurements of surface reflectance in various locations worldwide may not be a universal tool for satellite surface product validation. Given this, satellite surface products may suffer from aerosol contamination or lack of multiangle measurements for BRDF characterisation. In the frame of the ESA GROSAT project an essential GRaCE (G-band Radar for Cloud Experiments). University of Leicester presented the first measurements enhancement of the surface retrieval accuracy is achieved by inverting simultaneously AERONET groundbased and satellite measurements from diverse space-borne instruments like PARASOL, SentineI-5P/ from these instruments confirming the potential of G-band Radars for sizing sub-millimeter crystals in TROPOMI, Sentinel-2 and Sentinel-3/OLCI. This synergetic retrieval from the combination of groundice clouds and raindrops in light rain. based and satellite measurements was implemented into GRASP algorithm.

5.5 Clouds & Water Vapour

DLR showed a general framework for replacing the radiative transfer models used in an inversion algorithm with a deep neural network (DNN) that offers sufficient accuracy while at the same time increases the processing performance by several orders of magnitude. DLR demonstrated how the framework is used for the operational cloud product of Sentinel-5P, but also Sentinel-4 and how future improvements of the algorithms, by means of adding new physical models (e.g. ice-clouds), can be integrated.

BIRA-IASB presented the quality assessment of three TROPOMI cloud products and the evolution of



University of Lille presented the potential but also limitations of thermal hyperspectral infrared sounders such as IASI or IASI-NG to retrieve ice cloud properties by using a representative dataset from the global operational short range forecast of the ECMWF. The team developed and tested an algorithm which allows to retrieve, from an optimal estimation approach, the cloud integrated ice water content and the cloud layer altitude by using IASI and IASI-NG measurements.

ENTICE is a proposed satellite with multiple frequency sub-mm microwave radiometers and a cloud Radar instrument, which aims at providing observations of clouds, coincident vertical profiles of cloud ice particle size, ice water content, and in-cloud humidity and temperature. Caltech presented simulated ENTICE measurements with five different scanning methods: nadir, forward pointing, side scanning, and













conical scanning for the radiometers, and nadir pointing for the Radar.

University of Baghdad investigated the effects of cloud cover on solar radiation types for selected stations in Iraq. The results showed that the relationship between TCC and Top is inverse for the three stations, where Basra and Mosul stations represent the highest correlation while Baghdad station represents the middle correlation. As well as the highest amount of TCC occurred in the winter and spring season.

LATMOS analysed water vapour data observed during 2003 - 2014 period over the tropical region using largescale circulation for 7 global climate models (CMIP6 framework) and the new global water vapour climate data CNR-IFAC showed the assessment of the performance of the water vapour isotopologue retrieval using records (CDR) generated within the ESA Water Vapour CCI+ project (WV cci). The ESA WV cci and the CMIP6 the spectral coverage and radiometric accuracy of the FORUM observations, and the comparison with the data are then sorted according to dynamical regimes (intervals of 10 hPa/day) allowing to study the evolution results obtained when only the middle-infrared information is used. The retrieval is obtained by means of the Kyoto protocoL Informed Management of the Adaptation (KLIMA) retrieval code. Results on single of the regimes in terms of frequency of occurrence and is linked to water vapour variation. and averaged measurements evaluating the effect of the radiometric accuracy of the FORUM observations have been shown.

The Advanced Infra-Red WAter Vapour Estimator (AIRWAVE) algorithm has been investigated by CNR-ISAC to retrieve water vapour products from SLSTR on board Sentinel-3. AIRWAVE has the unique measurements to influence and possibly improve weather forecasts. capability to retrieve the TCWV over water surfaces for cloud-free scenarios using the SLSTR Thermal PicoSat presented the SATCROSS mission that aims at measuring the water vapour content in the lower Infrared channels, and therefore in both day- and night-time, covering all the water surfaces of the Earth. Performances of the AIRWAVE algorithm applied to SLSTR and validation performed with independent troposphere. In the basic configuration, a train of transmitting and receiving satellites is placed along the same orbit in such a way their line of sight passes tangentially to the Earth atmosphere, at altitudes below 10 km. products derived from space-borne sensors were discussed. A couple of very close radiofrequency (RF) K-band signals, emitted by a transmitting satellite to a receiving The newly developed retrieval of water isotopologues for Sentinel-5P based on the University of Leicester one, are attenuated while crossing the troposphere: such attenuations are then processed in order to recover two-dimensional water vapour fields on vertical sections of the troposphere itself.

Full Physics retrieval algorithm provides a dataset to study the distribution and changes of δD on high spatial and temporal resolution. University of Bergen compared the Sentinel-5P δD retrievals against in-situ vertical profiles of δD from the L-WAIVE campaign in June 2019 and model simulations with the A novel technique to measure water vapour in the lower troposphere has been developed by the University of isotope-enabled weather prediction model COSMOiso. Florence. The so-called NDSA is based on measurements of differential attenuation of two continuous tones

Atmos 2021 – Conference Report and User Recommendations

Caltech presented an assessment of the representation of clouds and water vapour structures in 28 climate models that participate in the Coupled Model Intercomparison Project Phase 6 (CMIP6) by means of NASA satellite data. Caltech found measurable improvements in CMIP6 models relative to CMIP5 models for both clouds and water vapour. The differences between models and satellite observations and the spread across the models are reduced.

SATCROSS is an ongoing project funded by ASI that aims at assessing the impact of water vapour estimates retrieved by Normalised Differential Spectral Attenuation (NDSA) measurements from co-rotating small LEO (Low Earth Orbit) satellites. In the framework of this project, LAMMA evaluated the capabilities of such new











demonstrator of such a technique operating in a ground-to-ground link configuration.

transmitted at 18.8 and 19.2 GHz on a line of sight radio link. The team reported on the results of the first EC-Earth climate model and the climatology built from ten years of IASI observations represents a very high confidence test for the direct verification and improvement of the global circulation models. University of Florence investigated the inversion problem relating to the acquisition system studied in the CNR-INO presented a fast and flexible Bayesian inversion model based on -FORUM with the capabilities SATCROSS project and further discussed inversion methods needed to achieve the spatial distribution of the of performing the synergistic inversion of both FORUM and IASI-NG measurements and to apply various water vapour. The specific geometry of the inversion problem at hand perfectly fits the so-called external types of constraints in the inversion, such as Optimal Estimation and/or Tikhonov regularisation. The reconstruction problem (ERP). following set of parameters can be retrieved: temperature, water vapour and ozone profiles, surface temperature and surface spectral emissivity.

Further, water vapour estimates provided by the NDSA in the 17-21 GHz frequency range are affected by a positive bias which is proportional to the total Integrated Liquid Water (ILW) content along the radio link. In the framework of SATCROSS project University of Florence proposed the use of the power ratio of the received signals at 31.8 GHz and at 16.9 GHz for directly estimating the path integrated liquid water content.

5.6 FORUM & Infrared Observation

University of Bologna showed preparatory studies for FORUM the 9th ESA Earth explorer mission. Specifically the team introduced a focus on the Chou's approximation, and a simple scaling method based on the similarity principle. The former one is widely implemented in existing fast radiative codes to solve the radiative transfer problems in the infrared spectral region considering a collection of atmospheric scenarios. In case of both water and ice cloud scenarios, the approximate solution performs well in the mid infrared for most of the cases studied.

A comparison between existing IASI observations against synthetic radiances extracted from the EC-Earth GCM (version 3.3.2) has been carried out by CNR-IFAC. Simulations provided by the EC-Earth model equipped with the new COSP + -FORUM module have been performed with prescribed sea surface temperature and sea-ice cover every 6 hours. The comparison between nadir radiances simulated by the

Atmos 2021 – Conference Report and User Recommendations

In preparation for the FORUM-EE9 mission, the analysis of the consistency between observations from prototypes of the FORUM Fourier Transform Spectrometer with similar spectral resolution and noise performance can be a first step toward an improvement of the water vapour spectroscopic data. CNR-ISAC exploit the balloon-borne measurements from the Radiation Explorer in the Far InfraRed -Prototype for Applications and Development (REFIR-PAD) and aircraft observations above the North Sea from the Tropospheric Airborne Fourier Transform Spectrometer (TAFTS) to assess the performances of different spectroscopic databases (HITRAN, AER, GEISA), coupled to different water vapour continuum parametrizations.

CNR-IAC showed how the FORUM instrument characteristics and the observed scene conditions impact the spectrum measured by the instrument, accounting for the main sources of error related to the entire acquisition process, and the consequences on the retrieval algorithm. The far-infrared part of the FORUM spectrum is shown to be sensitive to surface emissivity, in dry atmospheric conditions, and to cirrus clouds, resulting in improved performance of the retrieval algorithm in these conditions, while the retrieval errors increase with increasing the scene heterogeneity.

A comparison between two alternative approaches to determine atmospheric and surface state parameters, such as profiles of water vapour and temperature, surface temperature and spectral emissivity, by











exploiting simultaneously both FORUM and IASI-NG measurements has been carried out by CNR-INO. Daily TROPOMI Level 2 SO, data have been used to analyse the changes in the degassing behaviour in The team examined the synergistic retrieval of state parameters from the simultaneous inversion of both the periods before, during and after the eruption of Nyiragongo. University of Manchester also applied Sentinel-1 SAR data to look for ground deformation patterns on the volcano and the surrounding areas. measurements, and the a posteriori combination, via the Complete Data Fusion method, of the state The SO₂ flux time series shows a slight increase in degassing the days before the eruption while no parameters retrieved from the individual measurements. CNR-INO found that the exploitation of IASI-NG deformation is visible in the pre-eruptive interferograms. measurements would significantly improve the quality of FORUM retrieval products.

In the frame of the ESA DeepLIM project, Generative Adversarial Networks (GANs) and Autoencoders (AE) models are used to simulate Thermal Infra-Red (TIR) spectra acquired by satellite-borne instruments. CNR presented the characteristics (e.g. average values, standard deviations) of the generated dataset and compared them to the original ones highlighting the capability of deep learning techniques to support missions and retrieval algorithm development.

5.7 Volcanic Emissions

The discrepancy between TROPOMI and ground-based estimates conducted by the USGS at the Hawaii Volcano Observatory using a portable UV spectrometer of SO₂ emissions from Kilaurea eruption has been discussed by the University of Manchester. It was found that the flux was calculated using different wind speeds, the remote sensing one was measured by the Global Data Assimilation System and the other with an anemometer. A conclusion is that when both use the same wind speeds the fluxes are similar.

University of Manchester developed a new toolkit which allows the height and age of volcanic gas emissions to be quantified for each pixel containing a volcanic plume in a TROPOMI SO, image. PlumeTraj Combined observations of SO₂ measured by TROPOMI with PlumeTraj, a back-trajectory analysis toolkit, to reconstruct the hourly emission time-series during the onset of the explosive activity at La Soufrière is able to quantify the temporal evolution of explosive eruptions, the combination of mass eruption rate have been presented by University of Manchester. Their results highlighted the ability of satellite remote and gas emission rate allows to quantify the gas content within the magma which powers the eruption, sensing for investigating volcanic processes when combined with other analysis tools. This is especially a key parameter to understand volcanic processes. PlumeTraj allows strongly degassing volcanoes' flux the case when estimations of gas emissions cannot be measured from the ground, such as during to be quantified daily/hourly, complementing ground-based monitoring. explosive eruptions.

Atmos 2021 – Conference Report and User Recommendations



University of Tor Vergata presented the retrievals of volcanic ash detection in near real time mode by means of neural networks trained with MODIS data and applied to Sentinel-3/SLSTR measurements for the Raikoke eruption. The output of the approach is an image fully assigned to eight classes: ash over sea, over land and over clouds, sea, land and ice surfaces, weather ice and water vapour clouds. The results of the classification are consistent and promising, further developments are under consideration in order to improve the NN accuracy and ability to generalise even over other eruptive scenarios.

The location and strength of SO₂ emissions from Kilauea have been determined by Max Planck Institute using the divergence of the temporal mean SO_2 flux, an approach based on the continuity equation. Emission maps of SO₂ can be derived by the combination of satellite measurements and wind fields on high spatial resolution showing slightly lower estimates than the ones reported from ground-based measurements.









Inter-comparison and validation of SO₂ layer height from UV/Vis sensors against independent datasets, to four low-earth-orbit UV/Vis spectrometers: GOME/ERS2, SCIAMACHY/Envisat, GOME-2/METOPA and of a combined principle component analysis and a neural network retrieval algorithm called 'Full-Physics' OMI/AURA. Retrieval algorithms have been homogenised to ensure optimal consistency between the Inverse Learning Machine' has been shown by University of Thessaloniki. With respect to the previous historical QA4ECV dataset and the new TROPOMI operational products. algorithm it requires low computational resources and can be applied in near-real time.

5.8 Other Trace Gases and Atmospheric Processes

BIRA-IASB presented the first DOAS slant column retrieval results for HCHO from the Geostationary Environment Monitoring Spectrometer (GEMS) and compared the results to those from the polar orbiting sensor Sentinel-5P. The team focussed on the lessons learned from GEMS and how the algorithm developments performed in analysing GEMS data are beneficial for HCHO retrievals for the future Sentinel-4.

A novel machine learning approach, using an artificial neural network (ANN), is presented by University of Bremen in order to simulate enhanced tropospheric BrO in the Arctic. The ANN is a fast and computationally not demanding approach that can be integrated into chemical transport models as a sub-parameterization tool to predict the appearance of enhanced tropospheric BrO plumes quickly.

University of Leicester presented observations of HCN concentration over the Indonesia region measured by the Infrared Atmospheric Sounding Interferometer (IASI) instruments on-board the MetOp satellites during the Indonesian peatland fires from September to December 2015. For the same period HCN concentration is also investigated using an adapted version of the TOMCAT three-dimensional (3-D)

chemical transport model (CTM) and then compared with IASI retrievals. BIRA-IASB introduced the Cal/Val requirements identified for the constellation of Atmospheric Composition (AC) Sentinels being assembled: Sentinel-5P/TROPOMI, and the upcoming series of Sentinel-4 UVN, BIRA-IASB presented a 25-year multi-satellite data record of formaldehyde (HCHO) observations. Within Sentinel-5 UVNS, and CO2M. Emphasis is given to new Cal/Val challenges raised by the unprecedented the Quality Assurance for Essential Climate Variables (QA4ECV) project, a 20-year level-2 data record (1997spatial resolution of the Sentinels and the hourly sampling of diurnal changes in atmospheric composition. 2018) of HCHO columns was reprocessed using state of the art European retrieval algorithms applied Innovative approaches to improve the performance and optimise Cal/Val activities for the Sentinel

A tropospheric BrO column dataset covering the period 2007 to 2020 using GOME-2 measurements from Metop-A/B with the framework of the AC-SAF project has been generated by DLR. Some updates were included in the algorithm such as a new surface albedo database and an improved snow/ice flag compared to the scientific prototype algorithm. This algorithm is planned to be applied to TROPOMI measurements for the tropospheric BrO column retrieval, which makes it possible to extend the time series and monitor the spatiotemporal variability with a finer spatial resolution and a high signal to noise.

The circumpolar wind band (jet stream) represents a meridional barrier for air masses, but also energy fluxes. Planetary waves are well-known as main drivers of the large-scale weather patterns in midlatitudes on time scales from several days up to weeks in the troposphere. When planetary waves break, they often cut pressure cells off the jet stream. A specific example are so-called streamer events. In the framework of the LISA project DLR introduced a straightforward and robust method based on wind measurements and related quantities (vorticity, divergence) that reliably enables the detection of streamers in large data sets.

5.9 Calibration & Validation

Satellites were presented by ACRI-ST in the framework of H2020 project Copernicus Cal/Val soluti The project surveyed reference data used for calibration and validation, from on-board calibration devi to comparisons with models and other satellites, vicarious methods using natural scenes, as well systematic and campaign-based in-situ measurements.

GRASP-SAS presented the DIVA project (prototype) that is a hub to collect, handle, archive, and exploi a synergetic way observational data from ground and space that aims at validating ESA and Coperni satellite missions and scientific analysis. GRASP has been selected as the main algorithm to exp synergies of the data included in DIVA and retrieve advanced properties from the combination of sev instruments.

Max Planck Institute showed the new set-up of the high resolution regional atmospheric chemistry The status of Fundamental Data Record for ATMOSpheric Composition (FDR4ATMOS) project has been model WRF-Chem over western Europe and evaluated the NO₂ VCDs against TROPOMI observations. Very good initial model performance is observed if monthly mean spatial patterns of the simulated NO₂ shown by DLR. A full re-processing of the SCIAMACHY mission with the updated processor versions has been done, the validation showed that the total Ozone column drifted downward by nearly 2% over the VCDs are compared against TROPOMI observations while further adjustments had to be made in order to improve the agreement with daily measurements. mission lifetime. A next step of the FDR4ATMOS project is to develop a cross-instrument Level 1 product for GOME-1 and SCIAMACHY for the UV, Vis and NIR spectral range.

BIRA-IASB presented the first geophysical validation of GEMS Level-2 data products of NO₂, HCHO, and O₃ for four processed months (March to July 2021). The validation/evaluation methodology relies on the BIRA-IASB presented the major improvements implemented in the operational production of TROPOMI NO₂ data. The updates relate to the improved determination of cloud top pressure in the auxiliary analysis of data retrieval diagnostics and on comparisons with correlative measurements acquired by the FRESCO(-S) cloud retrieval and the use of profile information extracted from the CAMS-regional ensemble established ground-based instrument types: MAX DOAS, Zenith Scattered Light DOAS, Pandora, Fourier to replace that of the TM5 assimilation system. Essential in these assessments is the comparison to Multitransform infrared spectrometers (FTIR), Brewer, Dobson, and ozone sondes. Axis (MAX-) and Zenith-sky scattered light (ZSL-) DOAS measurement from the Network for the Detection

of Atmospheric Composition Change (NDACC), and to Pandonia Global Network (PGN) measurements. DLR developed a novel tomographic algorithm to allow for a three-dimensional reconstruction of the airglow layer by combining images from the two viewing angles. Multi-year observations of SABER on the TIMED-satellite are used on a statistical basis allowing to derive the vertical wavelength of the waves After more than 4 years in orbit, a combination of instrumental ageing and drift makes it necessary to update TROPOMI radiometric calibration key data also during the nominal operations phase. KNMI reported and see their three-dimensional structure. Tomographic reconstruction method has been explained which



ion.	on the in-flight calibration approach to characterise and differentiate between the various degra
ices	and drift effects. The observed optical degradation is most pronounced in the short wavelength
l as	of the instrument.
	The status of the architecture, data streams and functionalities of the Validation Data Analysis F (VDAF) and its Automated Validation Server (VDAF-AVS) with a focus on its application to Sentir
it in	has been presented by BIRA-IASB. TROPOMI and validation data are ingested and inter-compa
icus oloit eral	an automated validation system grounded on generic validation protocols and metrics, and implem using the Atmospheric Toolbox developed in heritage projects and tailored to the TROPOMI valion needs.











might in future also be applied on OH airglow image observations taken from satellite constellations.

The ESA atmospheric Validation Data Centre (EVDC) is the official ESA repository for calibration and validation (Cal/Val) data. Rhea Group showed the latest improvements of the platform such as the enhancement of the Cal/Val data filtering capabilities and search performance. Users are also now able to preview and inspect the contents of the Cal/Val files before downloading. The new ECMWF forecast data extraction and plotting tool is designed to simplify the access to the ECMWF forecasts.

The status of the first near-real-time (24h latency) central processing service for MAX-DOAS instruments, crucial for satellite products validation, has been shown by BIRA-IASB. Since November 2020, the processing system, which includes state-of-the-art retrieval algorithms, delivers on a daily basis tropospheric NO₂ vertical profile and total O₃ column data from 15 stations to the NDACC Rapid Delivery and ESA Validation Data Centre (EVDC) databases.

SERCO presented the Boundary-layer Air Quality-analysis Using Network of Instruments (BAQUNIN) supersite, which consists of three sites located in the city centre of Rome (Italy), and in the neighbouring semi-rural and rural areas. BAQUNIN has been promoted by ESA to establish an experimental research infrastructure for the validation of present and future satellite atmospheric products and the in-depth

A new blackbody, named Hemispherical Blackbody (HSBB), has been developed by Physikalisch-Technische investigation of the planetary and urban boundary layers. Bundesanstalt to allow accurate calibration of broadband infrared detectors having a hemispherical The opportunities offered through the joint Trans-National Access program of ACTRIS (Aerosol, Clouds acceptance angle. The aim is to develop a blackbody cavity with the same effective emissivity for normal and Trace gases Research InfraStructure), ICOS (Integrated Carbon Observation System) and IAGOS incidence and for the hemispherical opening angle in order to achieve consistency between measurements (In-service Aircraft for a Global Observing System) in the framework of the EC-funded ATMO-ACCESS with a radiation thermometer and detectors with a hemispherical opening angle.

project have been presented by National Institute of R&D for Optoelectronics. The project aims to collect specific technical and scientific needs and to identify and/or develop research and technology services in response to these needs. Key aspects that have been identified include: tailored measurement protocols, mobilised reference instruments for short-term campaigns, calibration services, developing and testing of new techniques, modules and algorithms, and addressing new synergies.

BIRA-IASB identified key challenges that complicate the validation of ex-ante uncertainties, and demonstrated how we can progress on that with applications of advanced methods to Sentinel-5P TROPOMI data. The team also discussed the gaps that are revealed in the ex-ante uncertainty characterization of both satellite and ground-based measurements, in particular regarding the differentiation between uncertainties associated with systematic and random effects.

In the framework of QA4EO project CNR-ISAC presented a new site in Po Valley compliant with the Fiducial Reference Measurements for Ground-Based DOAS (FRM4DOAS) standard. The objectives of the QA4EO are to demonstrate the importance of the DOAS measurements in the Po Valley, re-enforce the Italian know-how on MAX-DOAS technique and go towards the provision of standardised data for validation networks.











6. Recommendations to ESA

Recommendations to ESA collected during ATMOS-2021 are summarised in the table below.

ATMOS-2018 recommendations to ESA and related actions are summarised in the presentation: "Introduction to ATMOS-2021" by C. Retscher, Monday 2022-11-22, https://atmos2021.esa.int/iframe-agenda/files/Contribution_305_final_extabs.pdf.

	ATMOS-2021
	Air Qu
R1	Air quality space-based observations referred mainly to NO ₂ . Major progress is ex The amount of information should be maximised by combining datasets from in- dataset should also be considered in future studies. Beyond that, the potential o detection.
R2	TROPOMI NO ₂ observations are widely used for air quality monitoring at global a time series are available. The audience recommends a timely full reprocessing of

Atmos 2021 – Conference Report and User Recommendations



1 Recommendations

ality and Ozone

xpected on the simultaneous exploitation of NO₂ with other satellite products such as SO₂, aerosols and CO. -situ, ground-based remote sensing observations, as well as models. The advantages and limitations of each of AI should be further explored regarding e.g. dataset selection, retrieval methodology, and automated feature

and city scale. The most recent product update has shown some important improvements, but only parts of the f the product.





6. Recommendations to ESA

R3	 Two existing challenges require attention for further increasing the societal bene Robust and accurate methods for converting NO₂ column to surface concentra Health/exposure applications, particularly in urban areas, require even high instruments this could be achieved by further developing smart algorithms for synergies with other datasets/EO data/models, geostatistics, machine learning
R4	Establish a common basis for the understanding of the quality of the informati by using UV or UV/Vis and combined UV and TIR or other observations.
R5	ESA to establish scientific community activities on tropospheric ozone, as that is solar backscatter and thermal infrared EO data.
	Gree
R6	Gree Considering the Paris agreement and the record growth rate of $\mathrm{CH}_{\!_4}$ global concer
R6 R7	Gree Considering the Paris agreement and the record growth rate of CH ₄ global concer Further investigations on CH ₄ point sources are needed using collocated data from systematically analysed and include the assessment of uncertainties estimates.

Atmos 2021 – Conference Report and User Recommendations



fits of space-based AQ products and improve their utility for human exposure studies:

rations should be further developed (e.g. based on modelled surface-to-column ratios, machine learning, etc.) her-resolution satellite AQ products than those provided by TROPOMI. Aside from launching higher-resolution r increasing the spatial resolution and thus add value to the existing instruments (e.g. by oversampling techniques, ing)

ion i.e. the accuracy of the retrieved O_3 in the vertical profile, as a function of altitude in ozone nadir sounding

currently not adequately covered in CCI+ and other ESA programs. This could also include the synergistic use of

enhouse Gases

ntrations measured in 2020, there is a need to further study related processes by using satellite data.

m high resolution CH₄ missions. The monitoring of methane emission from these sources should be

ation using AI-based methods. This should be useful for CO2M and other higher resolution satellite missions





R9	Initial research on high resolution CH_4 observations from the Landsat series of processing procedures (e.g. automation of the plume detection, handling of false
R10	Further studies are needed for the detection and the quantification of CH_4 emission
R11	There is a need for additional ground-based CH ₄ observations to validate satellite
R12	Launch a study to support the understanding of 4D effects of CH ₄ plumes from swell as efforts on flux inversions (e.g. topography, AKs, wind).
R13	Regarding CH ₄ and CO ₂ products the continued (as done in GHG_cci) developmen shall be continued to be confronted.
R14	The audience highlighted the importance of building a European "facility-scale" (
R15	Regarding CO ₂ the importance of a continuous development of scientific and operation product from Sentinel-5, since relevant spectral bands are covered by the instrum
R16	The ongoing PRISMA and the future CO2M missions provide high resolution $\rm CO_2$ opre-eruption signals.



satellites is very promising. Support for further work is needed to improve the algorithms and streamline data positives). Further, the generation of a related historic dataset shall be studied.

ions at Northern latitudes related to thaw and freezing periods.

e products, especially at Northern latitudes

side of retrieval algorithms (e.g. shadowing, prior profiles, rerun retrieval with more info for identified images) as

it and maintenance of scientific products next to operational products is recommended. Ensembles of algorithms

 CH_4 and CO_2 satellite mission providing transparent and publicly available data products.

erational data products was highlighted. In this context, the audience specifically requested to develop an XCO₂ ment, but no operational product is currently planned.

observations. Further investigations are needed to explore the capabilities of these sensors to detect volcanic CO_2







	Sul
R17	Further studies are needed for the understanding of the discrepancies between s
R18	Radiative transfer and related assumptions shall be revisited, since the accuracy i
R19	 Regarding volcanic eruptions, the audience expressed the need for studies on foll For volcanic eruptions monitoring there is a need to provide more accurate m With respect to Neural Networks (NN) the ash classification should be further Near real time SO₂ plume height retrievals with improved sensitivity are need
R20	 Regarding aerosols, the audience expressed the need for studies on following aspective of the sensine of the sensine

Atmos 2021 – Conference Report and User Recommendations



phur Dioxide

space-borne and ground-based estimates of SO₂ emissions.

in the lower troposphere is limited, and a low SO_2 bias is suspected.

lowing aspects:

neasurements of sulphur dioxide (SO₂) in presence of large amounts of volcanic aerosols, especially ash. er improved by including more aerosols scenes (e.g. different types and measurement conditions). eded in order to improve plume dispersion modelling for detecting and tracking plumes from volcanic eruptions.

Aerosols

spects:

ng algorithms, aerosol retrievals over snow and ice shall be further studied;

ation nuclei and improve absorption (SSA) retrievals;

nes;

AOD scenarios since a systematic negative bias is observed in the validation against AERONET observations.





6. Recommendations to ESA

R21	ESA to establish scientific community activities on stratospheric aerosol profiles, synergistic use of active and passive EO data.
R22	Regarding the growing availability of aerosol data and products from Multi Angu single- or bi-viewing imagers. A large-scale activity such as Aerosol_cci would b as Angstrom Exponent, AODF, AODC, SSA, AAOD, etc. is needed.
R23	Beyond MAP prepare for future missions having the capability to measure aeroso products, which can also be validated with ground-based observations.
R24	Invest in the development and upgrade of advanced aerosol retrieval algorithms since this contributes to increasing coverage and reducing biases.
R25	Promote synergy of retrievals from various space-borne instruments to compens stratosphere). This allows to increase the information content, and therefore the
R26	ESA to further invest in synergetic retrievals from space-borne and ground-based from different satellites and will possibly facilitate new approaches for aerosol a
R27	The audience expressed a strong interest in the development of PM2.5 and PM1 aerosol observations also for non-scientific (e.g. policy makers) users. Investigat products. Investigate the synergy of satellite data and chemical transport model
R28	The validation of satellite surface products is challenging because there are no s AERONET for aerosols. Having these data at each AERONET site would be partice

Atmos 2021 – Conference Report and User Recommendations



as they are currently not adequately covered in CCI+ and other ESA programs. This could also include the

ular Polarimeters (MAP) instruments, the possibilities and needs are much broader compared to retrievals from De needed w.r.t. MAP data. Further support of data assimilation efforts on extended aerosol/MAP products such

ols such as EarthCARE, Aeolus follow-up, Sentinel-4, Sentinel-5, CO2M, and invest in well-defined aerosol

(e.g. GRASP, RemoTAP proven relevant for a large variety of sensors). Further invest in ensemble algorithms,

ate for individual weaknesses. Further bring aerosol communities together (e.g. IR, UV, troposphere, quality of the retrievals.

d instruments. This shall support the construction of a surface reference database for validation surface retrieval and surface modelling.

LO products from satellite data. If reliable, these retrievals might significantly increase the value of space-borne the synergistic retrievals using both in-situ and satellite data for constraining and improving the PM satellite Is, since this possibly presents a good combination for generating advanced PM products.

standard validation sources. There is a need to develop a global database for surface reflectance data such as Jularly useful for a comprehensive validation of satellite products.







R29	Assimilation of satellite products always comes with a necessary bias correction More effort is needed to support both communities to overcome this issue, impr
R30	 The audience expressed the need to further study cloud shadow and 3D cloud effects on a validated cloud shadow (fraction) product is satellite- and ground-based measurements. The impact of 3D cloud shape and cloud shadow on cloud retrievals; The 3D cloud effects on aerosol retrievals close to clouds edges; Cloud shadow impacts on CO₂ and CH₄ may be important and mitigation measurements.
R31	The audience highlighted the importance of cloud height knowledge. The choice algorithm version number can lead to noticeable differences. Work on cloud retri
R32	There is still some discrepancy between cloud products in the polar regions over phase cloud. More needs to be invested in this respect.
R33	There are some new products in extracting cloud microphysics from the IR spec
R34	Spectral line databases (e.g. HITRAN) and water vapour continuum representation further spectroscopic database improvements are required though.



n, due to the inconsistent radiative assumptions among the different models (surface, aerosols, clouds, etc.). Troving the consistency of the products (thus reducing the bias) or directly assimilating radiances.

Clouds

ffects. This should include:

needed. Cloud shadow effects on trace gas retrievals should be observationally verified preferably by combining

thods are needed for accurate measurements of anthropogenic emissions.

of cloud retrieval algorithm can have a considerable impact on trace gas retrievals, e.g., where a change of ieval algorithms deserves to be studied further.

r land and ocean for many satellite instruments and it is important to consider vertical structure and mixed

tral domain. This has a potential to be studied further specifically in polar regions in winter.

ons appear to generally be improving agreement between model and observations. More observations and







	Terre
R35	A request for the continued generation of SIF products from hyperspectral instru- include an effort on instrument intercalibration.
	Calibrati
R36	 On Cal/Val the audience requested support for ground-based observations that a Make use of trans-national research infrastructures and data sets for multiple instrumentation and fixed observatories) and co-design activities such as more coordinate between different ground-based networks to report uncertainties Harmonise reference datasets from networks such as TCCON and MUSICA-NI Further advanced platforms that provide access to diverse data and advance
R37	ESA shall continue to play an active role in Cal/Val activities for atmospheric Sen
R38	ESA to initiate and support (airborne) campaigns in relation to emission quantific become one of the most important products from atmospheric EO in air pollution input parameters (and source of errors). It is recommended that ESA initiates a

Atmos 2021 – Conference Report and User Recommendations



ments (as demonstrated for e.g. Sentinel-5P) and also for future missions has been expressed. This should also

ion and Validation

are crucial for any satellite product comparison activities. The following aspects should be addressed: le Cal/Val projects or campaigns. Foster collaboration across organisations to access facilities (mobile easurements campaigns and training;

in a similar way, considering both random and systematic values; DACC;

ed possibilities for using and visualising data in Cal/Val activities.

itinels (Sentinel-4, Sentinel-5, CO2M) to support campaigns to maximise the scientific use of those missions.

cation on different scales verifying/validating related satellite derived emission products, as emissions will n as well as for greenhouse gases. In this context the knowledge of the wind field is one of the most important measurement campaign with combined trace gas imager and wind LIDAR on ideally one aircraft.









	Ear
R39	When developing new data products for ESA Earth Explorers, a close link to the measurement information content.
R40	A monthly-mean L2A product (L3) should be developed from Aeolus retrievals. T be developed and applied before comparison.
R41	Through the synergy of L2A and L2B products, Aeolus provides the means to un and climate. A study mobilising expertise in Aeolus observations, state-of-the-ar climate modelling, could provide a complete assessment on the multifaceted clim

Atmos 2021 – Conference Report and User Recommendations



rth Explorers

DISC teams is recommended to further maximise expert input/feedback on data processing, quality and

This product should be compared to CALIPSO L3 to examine possible biases. A homogenization process should

nderstand the properties and lifetime of smoke particles in the stratosphere, as well as their impact on dynamics rt ground-based LIDAR microphysical retrievals, atmospheric radiative transfer, and comprehensive global matic relevance of stratospheric smoke.







6. Recommendations to ESA

	Missio
R42	 Beyond the already planned European missions, the audience raised the strategit troposphere to the lower thermosphere. This is part of a wider discussion of the research in environmental and climate change. In more detail, a strengthening of Tropospheric ozone from limb-nadir matching; Ozone-climate interaction and ozone recovery (e.g. NOy, HOy, BrOy, Ox); Monitoring upper atmospheric circulation in response to climate change (pass Long-term weather forecast (impact of stratosphere on tropospheric weather Stratosphere-troposphere exchange/UTLS (climate sensitive region); Stratospheric aerosols, i.e. impact of major/minor volcanic eruptions and pyr A redundancy of observations and a combination of observations in differented.
R43	ESA should increase its attention to commercial remote sensing, especially to the observations may be a highly valuable addition to conventional Earth Science observations of overall Earth observation and significantly help the scientific communant processing aspects in preparation of ESA's future missions. Therefore, ESA selected of private instruments in ESA missions, integrating small and medium develop a landscape that allows for maturing commercial satellite observations a

Atmos 2021 – Conference Report and User Recommendations



ns and Concepts

ic need for an adequate capability of space-based limb sounding of atmospheric composition from the upper e needs for a strategic European component in atmospheric composition monitoring as a key part of the of a continuous limb observation program is essential for:

ssive tracers: e.g. CO, N₂O, CH₄); er);

ro-fire events on climate; It spectral ranges (UV, Vis, IR, MW) is of great advantage.

the so-called "New Space" observations, which have been gradually appearing over recent years. These servations by ESA and other space agencies. Such observations may complement spatial coverage and temporal hity to further advance research. Commercial observations can also be used for testing various observational hall encourage the development of the private Earth Observation sector and markets by investing into the onsatellite observations produced by the private sector into the overall data provision. Beyond that ESA shall and reaching the quality standards of mainstream space observations.







