

# ATMOS-2021

## Conference Report and User Recommendations

Released on 2022-05-01

### Table of Contents

<b>1 Introduction</b>	<b>2</b>
<b>2 Objectives, Themes, Scientific Committee and Session Chairs</b>	<b>2</b>
<b>3 Plenary Sessions Summary &amp; Highlights</b>	<b>4</b>
3.1 Science from Space & Current Missions	4
3.2 Copernicus Services & Trainings	5
3.3 International Satellites, Missions and Products	6
3.4 Future Missions – Copernicus Sentinels	7
3.5 Future Missions – Earth Explorers & Earth Watch	8
3.6 Future Missions – Earth Explorer Candidates	9
3.7 The FORUM Mission	10
3.8 Aeolus Mission Data Exploitation	11
3.9 Air Quality	12
3.10 Ozone	14
3.11 Greenhouse Gases	16
3.12 Aerosols	19
3.13 Clouds	20
3.14 Water Vapour	21
3.15 Volcanic Emissions	22
3.16 OClO, BrO, Glyoxal	24
<b>4 e-Posters/Lightning Talks Sessions Summary &amp; Highlights</b>	<b>25</b>
4.1 Air Quality	25
4.2 Ozone	27
4.3 Greenhouse Gases	29
4.4 Aerosols & Surface	30
4.5 Clouds and Water Vapour	32
4.6 FORUM & Infrared Observations	34

4.7 Volcanic Emissions	35
4.8 Other Trace Gases and Atmospheric Processes	36
4.9 Calibration & Validation	37
<b>5 Recommendations to ESA</b>	<b>40</b>

## 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 Sentinel-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:

Number of participants	> 200
Number of thematic sessions	17
Number of oral presentations	101 + 2 keynote addresses
Number of e-Poster presentations	107

## 2 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 development and science activities regarding future missions, e.g

Copernicus Sentinel-4, Copernicus Sentinel-5, Copernicus CO<sub>2</sub>M, FORUM, EarthCARE, Altius, FLEX, TRUTHS and HARMONY;

- Provide updates on activities regarding ESA Third Party missions;
- Demonstrate the synergistic use of different atmospheric instruments;
- 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;
- 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;
- 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](http://atmos2018.esa.int/page_atmos2018_report.php));
- Provide a forum for scientists to formulate community recommendations.

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 Roozendaal (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 Roozendaal (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)

## 3 Plenary Sessions Summary & Highlights

### 3.1 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, OClO, H<sub>2</sub>O-ISO, SO<sub>2</sub>-LH, AOD/BRDF, SIF from Innovation projects and H<sub>2</sub>O, BrO from PAL project) are under finalisation and the upgrades to pre-operational 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 NO<sub>2</sub> 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.

## 3.2 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 composition, ocean, land hydrology & cryosphere, and land biosphere. All variables are available with long term and consistent time series that are constantly updated. A new set of web-based tools have been developed for the monitoring of climate change. This allows users to generate, in a traceable and reproducible way, Climate Indicators. These enable an operational monitoring on the long term evolution of several key variables used to assess the global and regional trends of warming climate such 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 enhanced ocean and land data assimilation.

CAMS combines information from Earth observation satellite and in-situ measurements, these inputs are processed using numerical models at global and regional scale and the outputs are provided to a wide range of users, from policy sector to commercial sector and air quality applications. Recently CAMS data has also been taken up by smartphone applications endorsed by the World Meteorological Application (WMO) and the European Environment Agency (EEA). CAMS has been renewed for another 7 years until 2028 and will increase the collaboration with the member states providing new

outputs related to pollutants and greenhouse gas fluxes. From October 2021, CAMS is assimilating tropospheric TROPOMI NO<sub>2</sub> measurements using also chemistry to account for the large NO<sub>2</sub> diurnal variability. The impact of this assimilation on surface NO<sub>2</sub> is small but reduces the NO<sub>2</sub> bias over China. The assimilation of SO<sub>2</sub> 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.

An overview of the training activities co-organized by ESA, EUMETSAT and ECMWF/CAMS has been presented. The so-called Joint Training on Atmospheric Composition provides lectures from top level scientists and hands-on support on dealing with atmospheric data. During the school events participants are encouraged to develop their own projects centred on the practical use of Copernicus (and related) data. Since 2019 more than 15 events (some organised only by EUMETSAT and ECMWF) have been co-organized also with specific sessions during conferences such as EGU. Beyond the school activities other initiatives like Massive On-line Courses (MOOC) have been organised. The latest iterations were on Artificial Intelligence for Earth Monitoring organised by Copernicus and on air quality monitoring during Covid-19 organised by ESA. Other provided training formats relate to thematically focused workshops such as the training schools on dust aerosol detection held in November 2021.

### 3.3 International Satellites, Missions and Products

NASA provided an overview of its latest developments regarding trace gases observations. A worldwide large decrease of NO<sub>2</sub> and SO<sub>2</sub> concentrations between 2005 and 2019 has been assessed by means of Ozone Monitoring Instrument (OMI) observations. A new series of products related to Volatile Organic Compounds (VOC) such as isoprene and a new ammonia product were retrieved in the IR band from IASI observations. The future geostationary mission TEMPO for the monitoring of atmospheric composition over North America and a dedicated validation campaign using also TEMPO simulated data held in September 2021 have been presented.

JAXA gave an overview of GOSAT and GOSAT-2 CO<sub>2</sub> measurements covering a total of twelve years of operation in space. Monthly maps of XCO<sub>2</sub>, XCH<sub>4</sub>, AOD and SIF are available from the JAXA website. During the Covid-19 pandemic these observations were provided to the trilateral ESA/NASA/JAXA EO-dash-board (<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 gas sensors has been introduced. Access to resources on the portal is free of charge and provides methodologies of vicarious calibration for various size footprint and off-nadir data, 13-year annual joint campaign data for Cal/Val and analytical results from various types of spectrometer such as GOSAT FTS, OCO and TROPOMI. In order to improve the estimates of global and local fluxes, JAXA developed a new imaging spectrometer for air-borne observations. Currently this is used on passenger aircrafts allowing the characterization of plumes producing fine scale CO<sub>2</sub> and NO<sub>2</sub> maps.

The new XCO<sub>2</sub> dataset from TanSat has been introduced by CAS. These data have been coupled with TROPOMI NO<sub>2</sub> 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/>. Global CO<sub>2</sub> 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 CO<sub>2</sub>, NO<sub>2</sub>, CH<sub>4</sub>, CO and SIF with a daily global coverage and a spatial resolution of 2x2 km<sup>2</sup> that can be increased to 500x500 m<sup>2</sup> 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 O<sub>3</sub>, NO<sub>2</sub>, SO<sub>2</sub>, HCHO, CHOCHO, AOD, AAI with spatial resolution of 3.5x8 km<sup>2</sup>. 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 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, CLONO<sub>2</sub>, HOCl and ClO have also been used to develop a climatology for inorganic chlorine (Cl<sub>y</sub>) 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.

### 3.4 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<sub>3</sub>, NO<sub>2</sub>, HCHO, CHOCHO, SO<sub>2</sub>, clouds and aerosols complemented by the operational AC-SAF products SO<sub>2</sub> layer height and H<sub>2</sub>O. 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).

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 CH<sub>4</sub>. 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 CO<sub>2</sub>M for the monitoring of anthropogenic CO<sub>2</sub> 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 push-broom 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 CO<sub>2</sub> missions filter out data for AOD>0.3, while CO<sub>2</sub>M 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. CO<sub>2</sub>M will provide CO<sub>2</sub>, CH<sub>4</sub>, NO<sub>2</sub> and SIF measurements with a 2x2 km<sup>2</sup> spatial resolution and aerosols with 4x4 km<sup>2</sup>.

For CO<sub>2</sub>M, 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.

### 3.5 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 NO<sub>2</sub> 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 consist 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.

### 3.6 Future Missions – Earth Explorer 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 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  $\text{cm}^{-1}$  and a nominal sampling of 50x50  $\text{km}^2$ . 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  $\text{NO}_x$  and  $\text{NH}_3$ . 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  $\text{NO}_2$  and  $\text{NH}_3$  emissions and their temporal patterns, the impact of these 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  $\text{NH}_3$  and a visible imaging pushbroom spectrometer for  $\text{NO}_2$  with a spatial resolution at least of  $0.5 \times 0.5 \text{ km}^2$ .

### 3.7 The FORUM Mission

The FORUM mission will provide a highly accurate global dataset of spectrally resolved far-infrared 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  $1600 \text{ cm}^{-1}$  with  $0.5 \text{ cm}^{-1}$  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.

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  $400\text{--}600 \text{ cm}^{-1}$  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.

### 3.8 Aeolus Mission Data Exploitation

The assimilation of Aeolus L2B wind profiles into numerical dispersion models has been successfully 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 volcanic ash when the model is initialised with Aeolus wind observations.

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 of Aeolus wind biases. The Loon Balloon Network provides wind observations in the upper troposphere/lower stratosphere which offer a valuable reference dataset for Aeolus product quality assessment in the tropics. The comparison revealed a relatively good agreement on wind horizontal variability while for the 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.

Aeolus wind measurements allow the derivation of atmospheric wave structures and wind gradients above the oceans where the wind ground-based observations are sparse. DLR showed how the Aeolus detection of the planetary waves by means of the streamer events is a powerful instrument to infer 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 differences were reported for zonal bands with higher values at higher latitudes.

Dust aerosols are a key component of the Earth-Atmosphere system with impacts on atmospheric 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 the assimilations of Aeolus wind profiles. An analysis showed that for several cases, either with high or low aerosol conditions, the WRF predictive skills were improved when the regional simulations were initialised after the considerations of Aeolus wind assimilation.

KNMI showed how cloud and aerosol properties can be retrieved from the Atmospheric Laser Doppler 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.

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 fundamental link between LIDAR surface returns, sea slope variance and near surface wind over water. Retrieved AOD from the LSR was compared with collocated L2A Aeolus operational extinction profiles 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.

Two algorithms of the Level 2A processor that aim to retrieve the atmospheric optical properties from the 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.

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.

### 3.9 Air Quality

KNMI presented the inversion algorithm Daily Emissions Constrained by Satellite Observations (DECSO) which can derive  $\text{NO}_x$  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  $\text{NO}_x$  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  $\text{NO}_2$  plumes from container ships over the Mediterranean sea. The TROPOMI  $\text{NO}_2$  value in the plume is defined as a mean of the three highest value  $\text{NO}_2$  pixels that fall within a polygon, delimited by the ship's route for the past hour as well as expected plume displacement due to prevailing wind conditions. The information on wind and other meteorological parameters is obtained from the ERA-5 model. Next steps of this work will deal with maritime emissions of  $\text{SO}_2$  and aerosols.

An improved  $\text{NO}_2$  tropospheric product for TROPOMI over Europe has been developed by KNMI. The algorithm consists of three steps: the spectral fitting of the slant column, the separation of

stratospheric and tropospheric contributions, and the conversion of the slant column to a vertical column using an air mass factor (AMF) calculation. A directionally dependent STRatospheric Estimation Algorithm from Mainz (DSTREAM) is developed to correct for the dependency of the stratospheric NO<sub>2</sub> on the viewing geometry. Validation with ground-based MAX-DOAS showed a good agreement with an underestimation of about 20%.

The University of Edinburgh developed an analysis tool using a convolutional neural network (CNN) to identify plumes of NO<sub>2</sub> 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<sub>2</sub> 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<sub>2</sub> 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<sub>2</sub> distribution is impacted by buildings so a city-scale dispersion model is used to take these effects into account.

MPI developed a method to retrieve the divergence of horizontal flux of trace gases by using TROPOMI NO<sub>2</sub> observations coupled with a wind field from ECMWF. The method works very well for point sources where spatial gradients of NO<sub>2</sub> are particularly high. More than 400 locations identified as NO<sub>x</sub> 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 NO<sub>2</sub> observations for urban applications.

Column amounts of NO<sub>2</sub> variations over regions with strong responses to Covid-19 have been addressed by DLR using GOME-2 and TROPOMI NO<sub>2</sub> observations. Long term data sets were seasonally adjusted based on climatological seasonal variability and corrected for the wind speed. Drops in NO<sub>2</sub> were observed in China, US and Europe with a gradual rebound 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 NO<sub>x</sub> emissions were derived from TROPOMI NO<sub>2</sub> 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.



### 3.10 Ozone

Tropospheric ozone in discrete vertical layers was retrieved from OMI observations and compared with UKESM1 simulations by University of Cambridge. Using the OMI dataset was possible to identify model biases related to the differences between model and observations in lower stratospheric ozone trends. It was also possible to identify stratospheric transport of ozone into the troposphere as the main driver of the North Atlantic ozone variability such as the Arctic oscillation. It was clarified that trend discrepancies 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 elements.

UV satellite estimates of ozone are able to make high-quality estimates of stratospheric concentrations 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 stratospheric ozone. Large volumes of data are available from current satellite instruments such as OMPS 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 presented the MUltiSpEctra, MUlti-SpECies, MUlti-SEnsors (MUSES) retrieval algorithm being developed for the TRopospheric Ozone and its Precursors from Earth System Sounding (TROPESS) framework. This 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, 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 column and similar agreement between CrIS-TROPOMI and CrIS-MLS retrieval is found for stratospheric 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.

A 25 years tropospheric ozone time series for the tropical band (20S to 20N) based on convective cloud differential algorithm (CCD) was presented by DLR including data from SCIAMACHY, OMI, GOME-2A, GOME-2B, GOME-2C and TROPOMI. SCIAMACHY data are used as a reference and fitted as an offset and a trend correction to the data of other sensors. From this long term dataset a mean tropical trend of 0.9 DU/decade in the tropospheric ozone was detected. A second data record that combines total ozone columns from TROPOMI with BASCOE stratospheric ozone profiles has been presented. Both ozone 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.

Another presentation from DLR showed global and regional ozone trends from the GOME-type Total Ozone Essential Climate Variable (GTO-ECV) data record. GTO-ECV combines observations from a series of 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  $1^\circ \times 1^\circ$ . In the framework of ESA-CCI+ it has been further improved and expanded with new satellite sensors including TROPOMI on board Sentinel-5P. Spatial and seasonal distribution of trends and the correlation with explanatory variables used in the regression model were presented, showing apparent signs of ozone recovery.

University of Bremen presented global O<sub>3</sub> trends from 1979 to 2020 using different merged total ozone datasets from satellite and ground-based observations. The merged datasets include data from NASA MOD v8.7, NOAA Cohesive Data (COH) v8.7, Global Ozone Monitoring Experiment (GOME)-type Total 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 (WOUDC). Trends showed a slow ozone recovery in both hemispheres, the median near global ozone trend after 1996 was  $0.5 \pm 0.2$  ( $2\sigma$ ) %/decade, which is in absolute numbers roughly a third of the decreasing rate of  $1.4 \pm 0.6$  ( $2\sigma$ ) %/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  $1\text{--}4\%$  dec<sup>-1</sup> 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<sub>3</sub> 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  $2\text{--}4\%$  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 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 dynamics processes.

FMI presented monthly  $1 \times 1$  deg<sup>2</sup> global tropospheric ozone using a combination of total ozone columns from OMI and TROPOMI with stratospheric ozone columns datasets from several available limb-viewing instruments. A method for data homogenization was set up, which includes the removal of biases and a-posteriori estimation (validation) of random uncertainties, thus making the data from different instruments compatible with each other. The global distributions of tropospheric ozone exhibit 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) have been presented showing very good agreement with ground-based observations and with TROPOMI and GOME-2 observations.

BIRA-IASB presented an initial validation of the atmospheric ozone profiles retrieved from TROPOMI. The validation was carried out using a diagnostic dataset (DDS5) of fourteen preselected orbits that together collocate with more than one hundred ground-based correlative measurements. The validation methodology relied on the analysis of data retrieval diagnostics and on comparisons of TROPOMI data with ground-based measurements. The latter were acquired by ozonesondes, stratospheric ozone LIDARs, and tropospheric ozone LIDARs. Preliminary results showed a slight striping along the orbit and a bias below 10% in the troposphere.

### 3.11 Greenhouse Gases

Atmospheric carbon dioxide (CO<sub>2</sub>) and methane (CH<sub>4</sub>) 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 CO<sub>2</sub> and CH<sub>4</sub> 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 XCO<sub>2</sub>. FOCAL is a candidate algorithm for the upcoming CO<sub>2</sub>M mission. The new v3.0 of GOSAT/GOSAT-2 FOCAL is available with additional products to XCO<sub>2</sub> such as XCH<sub>4</sub>, XH<sub>2</sub>O, HDO (delta D) and XN<sub>2</sub>O. Validation with the TCCON network showed good results. It was clarified that the a-priori CO<sub>2</sub> vertical profiles are based on the novel SLIM model which is based on Carbon Tracker data in combination with growth rates. Regarding the N<sub>2</sub>O, 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<sub>4</sub> 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  $\text{CH}_4$  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 ( $\text{XCH}_4$ ) 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  $50^\circ\text{N}$  and evaluated the  $\text{XCH}_4$  biases at four high-latitude TCCON sites. The polar vortex equally affected the performances of both TROPOMI and TCCON stations, and 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  $\text{CH}_4$  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 ( $3.7 \text{ m}^2$ ) have been shown by Universitat Politècnica de València (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 ( $\text{NO}_x$ ) to carbon dioxide ( $\text{CO}_2$ ) 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  $\text{NO}_x$ -to- $\text{CO}_2$  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  $\text{NO}_x$  lifetime.

The impact of scattering related  $\text{XCO}_2$  uncertainties in  $\text{CO}_2\text{M}$  data on inferring  $\text{CO}_2$  fluxes from cities has been investigated by SRON. Synthetic  $\text{CO}_2\text{M}$  data were perturbed according to  $\text{XCO}_2$  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  $\text{XCO}_2$  enhancements due to higher emissions in China.

High latitudes pose significant challenges to reliable space-based observations of total column carbon dioxide ( $\text{XCO}_2$ ) because snow-covered surfaces absorb strongly in the near-infrared wavelengths coinciding with the  $\text{CO}_2$  absorption channels of the Copernicus Anthropogenic  $\text{CO}_2$  Monitoring ( $\text{CO}_2\text{M}$ ) Mission. FMI presented a feasibility study of  $\text{CO}_2$  retrievals over snow from simulated  $\text{CO}_2\text{M}$  radiances. The team evaluated results against the ground-based  $\text{XCO}_2$  retrievals from the Total Carbon Column Observing Network (TCCON), and identified the snow-covered satellite pixels using auxiliary snow coverage data. The full  $\text{CO}_2$  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  $\text{CO}_2\text{M}$  satellite mission will provide new capabilities of imaging  $\text{CO}_2$  and  $\text{NO}_2$  which enables a quantitative assessment of  $\text{CO}_2$  emissions at the scale of large point sources such as power plants. The  $\text{CO}_2$  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  $\text{CO}_2$  and  $\text{NO}_2$  images. The first technique is 'denoising', to suppress incoherent additive (not just Gaussian) noise in the  $\text{CO}_2$  and  $\text{NO}_2$  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 “ $\text{CO}_2\text{image}$ ” that will complement the suite of planned  $\text{CO}_2$  sensor able to detect small point sources with a spatial resolution of  $50 \times 50 \text{ m}^2$ . A fleet of  $\text{CO}_2\text{Image}$  sensors would be able to monitor roughly 80% of the  $\text{CO}_2$  emissions from coal-fired power plants worldwide. One mission design element relates to adjusting local overpass times in order to achieve the mission objectives considering the diurnal variability of turbulence, cloud cover, wind speed and uncertainty, and measurement geometry. First results suggest an advantage to measuring earlier in the day, in contrast to the afternoon overpass time of most current missions targeting greenhouse gases. The instrument will be able also to retrieve methane. DLR also clarified that it is



important to look closely at the boundary layer evolution relevant for measurements and models especially in early morning conditions.

Total column concentrations of GHGs and other climate relevant gases retrieved from ground-based solar absorption measurements using Fourier transform infrared (FTIR) spectrometers used in the Total Carbon Column Observing Network (TCCON) are a primary source of reference data for validating satellite data. Instruments sample the whole atmospheric column, similar to the satellites. BIRA-IASB presented portable low-resolution FTIRs, one of which is the EM27/SUN that is used by the Collaborative Carbon 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 Politècnica 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.

### 3.12 Aerosols

DLR presented an ensemble algorithm for AOD applied within the Copernicus Climate Change Service (C3S) to several sensors: AATSR (and ATSR-2), SLSTR, OLCI and IASI. This algorithm uses the pixel-level uncertainties of several algorithms for the same sensor. Before calculating the ensemble results, the pixel-level uncertainties of all algorithms/instruments were evaluated against true errors versus AERONET. Validation of gridded daily ensemble products showed clear beneficial effects for the IASI ensemble, slight effects for ATSR-2 and SLSTR and limited impact for OLCI.

In the 2020s a number of satellites with Multi-Angle Polarimetric (MAP) instruments will be launched. KNMI showed the great potential of these polarisation sensitive sensors to retrieve high quality information on aerosol optical properties (size distribution, refractive index, shape). In the framework of the HARPOL project two full inversion algorithms (GRASP and RemoTAP) have been presented identifying for each of them strong/weak points and suggesting the optimized approach to retrieve aerosol properties. As it was noted, the objective of the HARPOL project is to suggest the potential optimizations of aerosol 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 presented an innovative framework for aerosol and surface retrievals from TROPOMI. It integrates the advanced Generalised Retrieval of Aerosol and Surface Properties (GRASP) algorithm and the heritage AOD and directional Lambertian equivalent reflectivity (DLER) algorithms. Results from validation of AOD and aerosol properties showed a very good agreement with AERONET surface observations and a fair agreement at global scale with well-validated aerosol and surface products from MODIS and VIIRS.

More insight into the Sentinel-5P +Innovation AOD/BRDF DLER algorithm has been provided by KNMI showing substantial improvements on the surface characterization evaluated by using TROPOMI geometry observation. The new LER products were integrated as ancillary information in the GRASP algorithm providing state-of-art aerosols and surface characterization including Angstrom exponent, single scattering albedo and surface BRDF and DLER.

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.

### 3.13 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 data and Sentinel-4 synthetic data have been provided. In the latest algorithm versions, the surface albedo climatology has been replaced with TROPOMI daily albedo retrievals (GE\_LER) and a detection flag is added to identify ice clouds. It was clarified that the ice flagging uses a simple threshold approach using CRB height and temperature profile from ECMWF.

Arctic amplification describes the recent period in which temperatures are rising twice as fast as the global average producing effects on Arctic's reflectivity that is dependent on the ice shelf and to the presence of clouds. DLR presented an investigation of the changes in the spectral reflectance at the

top of the atmosphere ( $R_{toa}$ ) 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 where the reflectivity diverges. While darkening areas can be attributed to seasonal sea ice decline, an 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 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  $NO_2$  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  $NO_2$  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.

### 3.14 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  $HDO/H_2O$ , 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.

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<sub>2</sub>O 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 rate changes with respect to surface temperature has been discussed. The available time series may not be long enough to make assumptions on a climate trend though.

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 characteristics of these CCI data records have been presented and related to other CDRs developed by NASA and NOAA. Multiple linear regression was applied to all time series to infer the seasonal cycle and a related disagreement has been discussed. It was underlined that not only the water millennium drop can be observed from all time-series but also another drop in 2014 needs to be further investigated.

### 3.15 Volcanic Emissions

Determining the height of SO<sub>2</sub> 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) SO<sub>2</sub> LH retrievals for SO<sub>2</sub> columns higher than 20 DU. The SO<sub>2</sub> layer height product has been validated successfully against IASI, OMI and CALIPSO observation and is actively assimilated by ECMWF/CAMS.

BIRA-IASB presented the Covariance-Based Retrieval Algorithm (COBRA), a new SO<sub>2</sub> LH algorithm based on TROPOMI observations that relies on an iterative approach making use of SO<sub>2</sub> optical depth look-up-tables. The major improvement of this algorithm relates to the sensitivity of the SO<sub>2</sub> LH product from 20 DU to 5 DU. Comparisons have been carried out with CALIOP, MLS and IASI observations for a number of volcanic eruptions showing an overall good agreement. However, a slight overestimation is observed for tropical eruptions at tropopause level and an underestimation for ash-laden plumes. The presence of 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.

Usually, horizontal homogenous atmospheric properties are assumed for the analysis of satellite observations of atmospheric trace gases causing only small errors in the retrievals. For volcanic plume retrieval this assumption leads to large errors. The Max Planck Institute for Chemistry (MPIC) investigated 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 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; c) saturation effects: for narrow plumes the SO<sub>2</sub> absorption signal can be strongly suppressed since most of the backscattered light is absorbed by SO<sub>2</sub> itself.

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/SO<sub>2</sub> molar ratio using TROPOMI observations following a DOAS algorithm approach. Calculated BrO/SO<sub>2</sub> ratios differ strongly between different volcanoes, variability for the same volcano is found at different points in time ranging from 10<sup>-5</sup> up to several 10<sup>-4</sup>.

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 observations. University of Manchester presented long-term averaging of TROPOMI observations of SO<sub>2</sub> columns retrieved with the COBRA algorithm. The Soufrière Hills volcano has been monitored using DOAS network data, while the plume is not visible from daily satellite imagery. Statistically, the west wind direction was prominent for 85-90% of the year. This is advantageous in the sense that gas will be blown in the same direction for most of the year, making the averaging technique more effective and making SO<sub>2</sub> plume visible also for TROPOMI. Before averaging a detailed SO<sub>2</sub> 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 SO<sub>2</sub> amount.



### 3.16 OClO, BrO, Glyoxal

The University of Bremen presented a novel algorithm for the retrieval of chlorine dioxide (OClO) from TROPOMI, developed in the framework of the Sentinel-5P +Innovation project. While OClO is not directly involved in stratospheric ozone depletion, it can serve as a quantitative indicator for stratospheric chlorine activation. The OClO 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 OClO data is a discontinuity originating from a new TROPOMI Level 1 dataset.

The MPIC presented a comparison between column densities of OClO 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. OClO SCDs also coincide well with CALIOP measurements for which PSCs are detected. Very high OClO 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 OClO 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 ( $\text{BrONO}_2$ ) derived from MIPAS have been presented by KIT. Simulations with the EMAC (ECHAM/MESSy Atmospheric Chemistry) model of stratospheric  $\text{BrONO}_2$  have been conducted and showed a model underestimation of enhanced  $\text{BrONO}_2$  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  $\text{NO}_2$  and  $\text{O}_3$  observation from the same instrument. Events of bromine explosions have been found for spring 2019 and 2020.

Glyoxal ( $\text{CHOCHO}$ ) in the atmosphere originates from the oxidation of biogenic and anthropogenic non-methane volatile organic compounds (NMVOCs).  $\text{CHOCHO}$  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  $\text{CHOCHO}$  columns densities from TROPOMI. The algorithm has been extended also to other satellite nadir sensors such as OM, GOME-2A and 2-B in order to temporally expand the  $\text{CHOCHO}$  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.

## 4 e-Posters/Lightning Talks Sessions Summary & Highlights

### 4.1 Air Quality

DLR presented a study on the relation between economic development and air quality over the Po Valley looking primarily at NO<sub>2</sub> concentrations by means of ERS-2, Envisat, MetOp-A and MetOp-B observations. First significant relations, with fewer NO<sub>2</sub> pollution outbreaks, were found in 2008 caused by the global 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 altitude research stations deployed throughout the Alpine region. VAO aims to contribute to a better understanding of environmental processes in the Alpine region. Outcomes and results of the work will support decision makers by balancing economic, social and environmental interests in a sustainable way.

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

University of Punjab showed an assessment of the air quality over Pakistan by using Sentinel-5P observations. Maximum concentrations of CO, HCHO and SO<sub>2</sub> were found during summer, winter and pre-monsoon season, respectively. The concentration of SO<sub>2</sub> increases to about 135.7% and 165.6% over Quetta and Peshawar.

FMI estimated ground level NO<sub>2</sub> concentrations over Finland from TROPOMI using methods by Lamsal et al. (2008) and Cooper et al. (2020) based on the GEOS-Chem chemical transport model. FMI found that the method by Cooper et al. (2020), which includes a correction for the vertical distribution of NO<sub>2</sub> within the boundary layer, overall performs better than the method by Lamsal et al. (2008) with no such correction.

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 clear trend albeit intensifying efforts and control measures by EU and local authorities.

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 between satellite and surface concentrations need further studies.

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.

University of Thessaloniki used Sentinel-5P/TROPOMI NO<sub>2</sub> observations in order to estimate updated NO<sub>x</sub> 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 through a data assimilation technique. The findings were validated by comparing NO<sub>2</sub> surface simulations from both free and assimilated CTM model runs to NO<sub>2</sub> in-situ measurements from an air quality station 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 NO<sub>2</sub> 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 using TROPOMI NO<sub>2</sub> 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 able to differentiate the NO<sub>2</sub> 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, and other vessels.

BIRA-IASB investigated the NO<sub>2</sub> distribution in Flanders as recorded by ground-based concentration measurements, airborne data and remotely-sensed density columns, with the help of the high-resolution WRF-Chem chemical-transport model as a cross-comparison tool. Simulated NO<sub>2</sub> distributions are compared against values from monitoring stations in Flanders, vertical columns measured by an airborne hyperspectral imager APEX and spaceborne NO<sub>2</sub> columns obtained by TROPOMI.

Tropospheric NO<sub>2</sub> retrievals (Level-2) from TROPOMI have been used to observe the current state of NO<sub>2</sub> pollution and detect new hotspots in South Asia during July 2018 to September 2021 by University of Punjab. Also, a comparison of spatial distributions of NO<sub>2</sub> retrieved from TROPOMI and OMI has been 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 Gimbalbed 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 weeks before both measurements.

University of Oslo derived a spatially continuous surface NO<sub>2</sub> concentration from tree-based machine learning models such as Random Forest and Extreme Gradient Boosting (XGBoost), using datasets such as tropospheric NO<sub>2</sub> from TROPOMI, day-night band from the Visible Infrared Imaging Radiometer Suite (VIIRS) instrument, NO<sub>2</sub> station measurements from the European Environmental Agency (EEA) and secondary variables such as meteorological parameters and land use land cover information. The preliminary outputs of this work show promising results with a mean absolute error of 10.4 µ/m<sup>3</sup> and 12 µ/m<sup>3</sup> respectively for Random Forest and XGBoost models.

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 concentrations by means of a simple linear relation between ground level concentrations and the total column concentrations provided by satellite measurements.

Airborne in-situ measurements of sulphur dioxide (SO<sub>2</sub>) emissions plumes from two coal-fired power 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 problems with dense smoke clouds frequently covering these countries in winter. First estimates by means of a mass balance approach showed that the SO<sub>2</sub> mass flux from Tuzla is about twice as high as indicated by common emission inventories.

## 4.2 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.

CNRS presented a comprehensive study integrating satellite observations of ozone pollution in-situ measurements and chemistry transport model simulations for quantifying the role of anthropogenic emission reductions during the Covid-19 lockdown in spring 2020 over Europe. CNRS found clear 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 observed elsewhere, where ozone chemistry is limited by the abundance of NO<sub>x</sub>.

A complete characterization of the TROPOMI tropospheric ozone, providing clues to properly include it in 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 Dijkstra's algorithm, one of the candidates algorithm to solve this problem.

Surface ozone concentration in ambient air is influenced by background value, regional and local chemical 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 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.

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.

## 4.3 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 Politècnica de Valencia focused on the retrieval performance attending to factors such as the temporal misregistration, angular differences or spectral mismatch.

Several atmospheric CO<sub>2</sub> products, such as ACOS, NIES, OCFP and SRFP products from the full physics retrieval algorithm, provide CO<sub>2</sub> surface flux of GOSAT. In order to obtain the CO<sub>2</sub> data set with high precision, low uncertainty and high coverage, University of Mining and Technology used the products of the above four algorithms for fusion. Since the products of the same satellite are used, there is no need to consider the matching of time and space factors. The fusion results were encouraging, not only increasing the coverage of XCO<sub>2</sub>, but also demonstrating a good accuracy in validation with TCCON observations.

University of Bremen quantified the CO<sub>2</sub> emissions from localised sources such as power plants by using XCO<sub>2</sub> 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 NO<sub>2</sub> as a tracer for recently emitted CO<sub>2</sub> and an inversion technique to quantify CO<sub>2</sub> emissions from detected CO<sub>2</sub> plumes.

An algorithm to calculate CO<sub>2</sub> 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 CO<sub>2</sub> 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 XCH<sub>4</sub> 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 covering absorption bands of CO<sub>2</sub> and CH<sub>4</sub> between ~1575 and ~1700 nm with a spectral resolution of ~1.1 nm. It is designed to detect and quantify CO<sub>2</sub> and CH<sub>4</sub> emissions from point sources, and serves as precursor and demonstrator for the larger 2-channel imaging spectrometer MAMAP2D, which is currently in the development phase.

## 4.4 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 O<sub>2</sub>A 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 observations collected by MERIS, was conducted by DLR. The approach has three independent parts, i.e. the preprocessor, the associator and the trainer, whereby the data are significantly reduced in size, matched spatio-temporally with data from the Aerosol Robotic Network (AERONET) and are finally trained with a neural network.

The Aerosol Index (AI) retrieved from TROPOMI's high spatial resolution observations presents specific challenges as non-Lambertian cloud features, cloud shadows, and 3-D effects of clouds are now visible in 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-dependent degradation in the TROPOMI irradiance and radiance data.

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 that retrieves the particle backscatter coefficient, the particle extinction coefficient, and the linear and 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 Friday evening matching a close Aeolus overpass.

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 account for aerosol perturbation of in-cloud extinction profiles based on the synergistic exploitation of oxygen absorption and multi-wavelength continuum in the solar spectral range.

University of Thessaloniki analysed the impact of wildfires over Greece on atmospheric aerosol load using satellite data. A synergy of satellite data from GOME-2 and TROPOMI is used to derive the aerosol optical and geometrical properties, during biomass burning events observed over Greece in the 2021 summer fires. The measurements allowed the monitoring of the evolution of fresh smoke aerosols, as well as to analyse its optical and geometrical properties (horizontal and vertical extent).

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 by two-stream approximation was proposed by University of Mining and Technology. The team showed results of SSA inversions over China and successfully validated against 7 AERONET sites for April 2020.

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 XCO<sub>2</sub> retrieval only based on the high-resolution spectrometer for CO<sub>2</sub> measurements (CO2I) observations. The proposed approach uses the GRASP algorithm to infer aerosol properties from MAP measurements, and feeds its retrieved information to the UoL full physics CO<sub>2</sub> retrieval, which is based on optimal estimation.

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 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 are averaged within 0.5 degrees radius around ground-based LIDAR location.

DLR presented a novel algorithm for the retrieval of geometry-dependent effective Lambertian equivalent reflectivity (GE\_LER) from UVN sensors based on the full-physics inverse learning machine (FP\_ILM) retrieval. The GE\_LER retrieval is optimised for the trace gas retrievals using the DOAS algorithm and the large amount of data of the new atmospheric Sentinel satellite missions. The TROPOMI GE\_LER/G3\_LER results for the fitting windows corresponding to O<sub>3</sub>, NO<sub>2</sub>, SO<sub>2</sub>, HCHO, H<sub>2</sub>O, and clouds are presented and compared with climatological OMI and GOME-2 LER data.

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 multi-angle measurements for BRDF characterisation. In the frame of the ESA GROSAT project an essential enhancement of the surface retrieval accuracy is achieved by inverting simultaneously AERONET ground-based and satellite measurements from diverse space-borne instruments like PARASOL, Sentinel-5P/TROPOMI, Sentinel-2 and Sentinel-3/OLCI. This synergetic retrieval from the combination of ground-based and satellite measurements was implemented into GRASP algorithm.

## 4.5 Clouds and 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 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 O<sub>2</sub> 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 GRaCE (G-band Radar for Cloud Experiments). University of Leicester presented the first measurements from these instruments confirming the potential of G-band Radars for sizing sub-millimeter crystals in ice clouds and raindrops in light rain.

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.

CNR-IFAC showed the assessment of the performance of the water vapour isotopologue retrieval using the spectral coverage and radiometric accuracy of the FORUM observations, and the comparison with the 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 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 capability to retrieve the TCWV over water surfaces for cloud-free scenarios using the SLSTR Thermal 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 products derived from space-borne sensors were discussed.

The newly developed retrieval of water isotopologues for Sentinel-5P based on the University of Leicester Full Physics retrieval algorithm provides a dataset to study the distribution and changes of  $\delta D$  on high spatial and temporal resolution. University of Bergen compared the Sentinel-5P  $\delta D$  retrievals against in-situ vertical profiles of  $\delta D$  from the L-WAIVE campaign in June 2019 and model simulations with the isotope-enabled weather prediction model COSMOiso.

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.

LATMOS analysed water vapour data observed during 2003 - 2014 period over the tropical region using large-scale circulation for 7 global climate models (CMIP6 framework) and the new global water vapour climate data records (CDR) generated within the ESA Water Vapour CCI+ project (WV\_cci). The ESA WV\_cci and the CMIP6 data are then sorted according to dynamical regimes (intervals of 10 hPa/day) allowing to study the evolution of the regimes in terms of frequency of occurrence and is linked to water vapour variation.

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 measurements to influence and possibly improve weather forecasts.



PicoSat presented the SATCROSS mission that aims at measuring the water vapour content in the lower 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. A couple of very close radiofrequency (RF) K-band signals, emitted by a transmitting satellite to a receiving 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.

A novel technique to measure water vapour in the lower troposphere has been developed by the University of Florence. The so-called NDSA is based on measurements of differential attenuation of two continuous tones transmitted at 18.8 and 19.2 GHz on a line of sight radio link. The team reported on the results of the first demonstrator of such a technique operating in a ground-to-ground link configuration.

University of Florence investigated the inversion problem relating to the acquisition system studied in the SATCROSS project and further discussed inversion methods needed to achieve the spatial distribution of the water vapour. The specific geometry of the inversion problem at hand perfectly fits the so-called external reconstruction problem (ERP).

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.

## 4.6 FORUM & Infrared Observations

University of Bologna showed preparatory studies for FORUM the 9<sup>th</sup> 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 +  $\sigma$ -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 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.

CNR-INO presented a fast and flexible Bayesian inversion model based on  $\sigma$ -FORUM with the capabilities of performing the synergistic inversion of both FORUM and IASI-NG measurements and to apply various types of constraints in the inversion, such as Optimal Estimation and/or Tikhonov

regularisation. The following set of parameters can be retrieved: temperature, water vapour and ozone profiles, surface temperature and surface spectral emissivity.

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. The team examined the synergistic retrieval of state parameters from the simultaneous inversion of both measurements, and the a posteriori combination, via the Complete Data Fusion method, of the state parameters retrieved from the individual measurements. CNR-INO found that the exploitation of IASI-NG 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.

## 4.7 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 SO<sub>2</sub> emissions from Kilauea 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.

Combined observations of SO<sub>2</sub> 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 have been presented by University of Manchester. Their results highlighted the ability of satellite remote sensing for investigating volcanic processes when combined with other analysis tools.

This is especially the case when estimations of gas emissions cannot be measured from the ground, such as during explosive eruptions.

Daily TROPOMI Level 2 SO<sub>2</sub> data have been used to analyse the changes in the degassing behaviour in 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. The SO<sub>2</sub> flux time series shows a slight increase in degassing the days before the eruption while no deformation is visible in the pre-eruptive interferograms.

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 SO<sub>2</sub> emissions from Kilauea have been determined by Max Planck Institute using the divergence of the temporal mean SO<sub>2</sub> flux, an approach based on the continuity equation. Emission maps of SO<sub>2</sub> 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.

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<sub>2</sub> image. PlumeTraj is able to quantify the temporal evolution of explosive eruptions, the combination of mass eruption rate and gas emission rate allows to quantify the gas content within the magma which powers the eruption, a key parameter to understand volcanic processes. PlumeTraj allows strongly degassing volcanoes' flux to be quantified daily/hourly, complementing ground-based monitoring.

Inter-comparison and validation of SO<sub>2</sub> layer height from UV/Vis sensors against independent datasets, of a combined principle component analysis and a neural network retrieval algorithm called 'Full-Physics Inverse Learning Machine' has been shown by University of Thessaloniki. With respect to the previous algorithm it requires low computational resources and can be applied in near-real time.

## 4.8 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 presented a 25-year multi-satellite data record of formaldehyde (HCHO) observations. Within the Quality Assurance for Essential Climate Variables (QA4ECV) project, a 20-year level-2 data record (1997-2018) of HCHO columns was reprocessed using state of the art European retrieval algorithms applied to four low-earth-orbit UV/Vis spectrometers: GOME/ERS2, SCIAMACHY/Envisat, GOME-2/METOPA and OMI/AURA. Retrieval algorithms have been homogenised to ensure optimal consistency between the historical QA4ECV dataset and the new TROPOMI operational products.

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 mid-latitudes 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.

## 4.9 Calibration & Validation

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, Sentinel-5 UVNS, and CO2M. Emphasis is given to new Cal/Val challenges raised by the unprecedented spatial resolution of the Sentinels and the hourly sampling of diurnal changes in atmospheric composition.

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

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

The status of Fundamental Data Record for ATMOSpheric Composition (FDR4ATMOS) project has been 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 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 major improvements implemented in the operational production of TROPOMI NO<sub>2</sub> data. The updates relate to the improved determination of cloud top pressure in the auxiliary FRESCO(-S) cloud retrieval and the use of profile information extracted from the CAMS-regional ensemble to replace that of the TM5 assimilation system. Essential in these assessments is the comparison to Multi-Axis (MAX-) and Zenith-sky scattered light (ZSL-) DOAS measurement from the Network for the Detection of Atmospheric Composition Change (NDACC), and to Pandora Global Network (PGN) measurements.

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 on the in-flight calibration approach to characterise and differentiate between the various degradation and drift effects. The observed optical degradation is most pronounced in the short wavelength range of the instrument.

The status of the architecture, data streams and functionalities of the Validation Data Analysis Facility (VDAF) and its Automated Validation Server (VDAF-AVS) with a focus on its application to Sentinel-5P has been presented by BIRA-IASB. TROPOMI and validation data are ingested and inter-compared in an automated validation system grounded on generic validation protocols and metrics, and implemented using the Atmospheric Toolbox developed in heritage projects and tailored to the TROPOMI validation needs.

Max Planck Institute showed the new set-up of the high resolution regional atmospheric chemistry model WRF-Chem over western Europe and evaluated the NO<sub>2</sub> VCDs against TROPOMI observations. Very good initial model performance is observed if monthly mean spatial patterns of the simulated NO<sub>2</sub> VCDs are compared against TROPOMI observations while further adjustments had to be made in order to improve the agreement with daily measurements.

BIRA-IASB presented the first geophysical validation of GEMS Level-2 data products of NO<sub>2</sub>, HCHO, and O<sub>3</sub> for four processed months (March to July 2021). The validation/evaluation methodology relies on the analysis of data retrieval diagnostics and on comparisons with correlative measurements acquired by the established ground-based instrument types: MAX DOAS, Zenith Scattered Light DOAS, Pandora, Fourier transform infrared spectrometers (FTIR), Brewer, Dobson, and ozone sondes.



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 and see their three-dimensional structure. Tomographic reconstruction method has been explained which 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 NO<sub>2</sub> vertical profile and total O<sub>3</sub> 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 investigation of the planetary and urban boundary layers.

The opportunities offered through the joint Trans-National Access program of ACTRIS (Aerosol, Clouds and Trace gases Research InfraStructure), ICOS (Integrated Carbon Observation System) and IAGOS (In-service Aircraft for a Global Observing System) in the framework of the EC-funded ATMO-ACCESS 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.

A new blackbody, named Hemispherical Blackbody (HSBB), has been developed by Physikalisch-Technische Bundesanstalt to allow accurate calibration of broadband infrared detectors having a hemispherical acceptance angle. The aim is to develop a blackbody cavity with the same effective emissivity for normal incidence and for the hemispherical opening angle in order to achieve consistency between measurements with a radiation thermometer and detectors with a hemispherical opening angle.

## 5 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](https://atmos2021.esa.int/iframe-agenda/files/Contribution_305_final_extabs.pdf).

ATMOS-2021 Recommendations	
Air Quality and Ozone	
<b>R1</b>	Air quality space-based observations referred mainly to NO <sub>2</sub> . Major progress is expected on the simultaneous exploitation of NO <sub>2</sub> with other satellite products such as SO <sub>2</sub> , aerosols and CO. The amount of information should be maximised by combining datasets from in-situ, ground-based remote sensing observations, as well as models. The advantages and limitations of each dataset should also be considered in future studies. Beyond that, the potential of AI should be further explored regarding e.g. dataset selection, retrieval methodology, and automated feature detection.
<b>R2</b>	TROPOMI NO <sub>2</sub> observations are widely used for air quality monitoring at global and city scale. The most recent product update has shown some important improvements, but only parts of the time series are available. The audience recommends a timely full reprocessing of the product.
<b>R3</b>	Two existing challenges require attention for further increasing the societal benefits of space-based AQ products and improve their utility for human exposure studies: <ul style="list-style-type: none"> <li>• Robust and accurate methods for converting NO<sub>2</sub> column to surface concentrations should be further developed (e.g. based on modelled surface-to-column ratios, machine learning, etc.)</li> <li>• Health/exposure applications, particularly in urban areas, require even higher-resolution satellite AQ products than those provided by TROPOMI. Aside from launching higher-resolution instruments this could be achieved by further developing smart algorithms for increasing the spatial resolution and thus add value to the existing</li> </ul>

	instruments (e.g. by oversampling techniques, synergies with other datasets/EO data/models, geostatistics, machine learning)
<b>R4</b>	Establish a common basis for the understanding of the quality of the information i.e. the accuracy of the retrieved O <sub>3</sub> in the vertical profile, as a function of altitude in ozone nadir sounding by using UV or UV/Vis and combined UV and TIR or other observations.
<b>R5</b>	ESA to establish scientific community activities on tropospheric ozone, as that is currently not adequately covered in CCI+ and other ESA programs. This could also include the synergistic use of solar backscatter and thermal infrared EO data.
<b>Greenhouse Gases</b>	
<b>R6</b>	Considering the Paris agreement and the record growth rate of CH <sub>4</sub> global concentrations measured in 2020, there is a need to further study related processes by using satellite data.
<b>R7</b>	Further investigations on CH <sub>4</sub> point sources are needed using collocated data from high resolution CH <sub>4</sub> missions. The monitoring of methane emission from these sources should be systematically analysed and include the assessment of uncertainties estimates.
<b>R8</b>	ESA to trigger a study on the automatic CH <sub>4</sub> plume detection and source classification using AI-based methods. This should be useful for CO <sub>2</sub> M and other higher resolution satellite missions (e.g. PRISMA).
<b>R9</b>	Initial research on high resolution CH <sub>4</sub> observations from the Landsat series of satellites is very promising. Support for further work is needed to improve the algorithms and streamline data processing procedures (e.g. automation of the plume detection, handling of false positives). Further, the generation of a related historic dataset shall be studied.
<b>R10</b>	Further studies are needed for the detection and the quantification of CH <sub>4</sub> emissions at Northern latitudes related to thaw and freezing periods.
<b>R11</b>	There is a need for additional ground-based CH <sub>4</sub> observations to validate satellite products, especially at Northern latitudes.
<b>R12</b>	Launch a study to support the understanding of 4D effects of CH <sub>4</sub> plumes from side of retrieval algorithms (e.g. shadowing, prior profiles, rerun retrieval with more info for identified images) as well as efforts on flux inversions (e.g. topography, AKs, wind).
<b>R13</b>	Regarding CH <sub>4</sub> and CO <sub>2</sub> products the continued (as done in GHG_cci) development and maintenance of scientific products next to operational products is recommended. Ensembles of algorithms shall be continued to be confronted.
<b>R14</b>	The audience highlighted the importance of building a European “facility-scale” CH <sub>4</sub> and CO <sub>2</sub> satellite mission providing transparent and publicly available data products.
<b>R15</b>	Regarding CO <sub>2</sub> the importance of a continuous development of scientific and operational data products was highlighted. In this context, the audience specifically requested to develop an XCO <sub>2</sub> product from Sentinel-5, since relevant spectral bands are covered by the instrument, but no operational product is currently planned.
<b>R16</b>	The ongoing PRISMA and the future CO <sub>2</sub> M missions provide high resolution CO <sub>2</sub> observations. Further investigations are needed to explore the capabilities of these sensors to detect volcanic CO <sub>2</sub> pre-eruption signals.

Sulphur Dioxide	
<b>R17</b>	Further studies are needed for the understanding of the discrepancies between space-borne and ground-based estimates of SO <sub>2</sub> emissions.
<b>R18</b>	Radiative transfer and related assumptions shall be revisited, since the accuracy in the lower troposphere is limited, and a low SO <sub>2</sub> bias is suspected.
<b>R19</b>	Regarding volcanic eruptions, the audience expressed the need for studies on following aspects: <ul style="list-style-type: none"> <li>• For volcanic eruptions monitoring there is a need to provide more accurate measurements of sulphur dioxide (SO<sub>2</sub>) in presence of large amounts of volcanic aerosols, especially ash.</li> <li>• With respect to Neural Networks (NN) the ash classification should be further improved by including more aerosols scenes (e.g. different types and measurement conditions).</li> <li>• Near real time SO<sub>2</sub> plume height retrievals with improved sensitivity are needed in order to improve plume dispersion modelling for detecting and tracking plumes from volcanic eruptions.</li> </ul>
Aerosols	
<b>R20</b>	Regarding aerosols, the audience expressed the need for studies on following aspects: <ul style="list-style-type: none"> <li>• In order to work on a clear gap in current spaceborne aerosol remote sensing algorithms, aerosol retrievals over snow and ice shall be further studied;</li> <li>• Work on retrievals of aerosol chemical composition, size and cloud condensation nuclei and improve absorption (SSA) retrievals;</li> <li>• Study the effect of cloud screening and aerosol retrieval in partly cloudy scenes;</li> <li>• Develop aerosol-above-cloud retrievals;</li> <li>• Develop and/or further enhance simultaneous aerosol and cloud retrievals;</li> <li>• Develop and/or further enhance simultaneous aerosol and surface retrievals;</li> <li>• Improve aerosol algorithms from different satellite sensor retrievals for high AOD scenarios since a systematic negative bias is observed in the validation against AERONET observations.</li> </ul>
<b>R21</b>	ESA to establish scientific community activities on stratospheric aerosol profiles, as they are currently not adequately covered in CCI+ and other ESA programs. This could also include the synergistic use of active and passive EO data.
<b>R22</b>	Regarding the growing availability of aerosol data and products from Multi Angular Polarimeters (MAP) instruments, the possibilities and needs are much broader compared to retrievals from single- or bi-viewing imagers. A large-scale activity such as Aerosol_cci would be needed w.r.t. MAP data. Further support of data assimilation efforts on extended aerosol/MAP products such as Angstrom Exponent, AODF, AODC, SSA, AAOD, etc. is needed.
<b>R23</b>	Beyond MAP prepare for future missions having the capability to measure aerosols such as EarthCARE, Aeolus follow-up, Sentinel-4, Sentinel-5, CO2M, and invest in well-defined aerosol products, which can also be validated with ground-based observations.
<b>R24</b>	Invest in the development and upgrade of advanced aerosol retrieval algorithms (e.g. GRASP, RemoTAP proven relevant for a large variety of sensors). Further invest in ensemble algorithms, since this contributes to increasing coverage and reducing biases.

<b>R25</b>	Promote synergy of retrievals from various space-borne instruments to compensate for individual weaknesses. Further bring aerosol communities together (e.g. IR, UV, troposphere, stratosphere). This allows to increase the information content, and therefore the quality of the retrievals.
<b>R26</b>	ESA to further invest in synergetic retrievals from space-borne and ground-based instruments. This shall support the construction of a surface reference database for validation surface retrieval from different satellites and will possibly facilitate new approaches for aerosol and surface modelling.
<b>R27</b>	The audience expressed a strong interest in the development of PM <sub>2.5</sub> and PM <sub>10</sub> products from satellite data. If reliable, these retrievals might significantly increase the value of space-borne aerosol observations also for non-scientific (e.g. policy makers) users. Investigate synergistic retrievals using both in-situ and satellite data for constraining and improving the PM satellite products. Investigate the synergy of satellite data and chemical transport models, since this possibly presents a good combination for generating advanced PM products.
<b>R28</b>	The validation of satellite surface products is challenging because there are no standard validation sources. There is a need to develop a global database for surface reflectance data such as AERONET for aerosols. Having these data at each AERONET site would be particularly useful for a comprehensive validation of satellite products.
<b>R29</b>	Assimilation of satellite products always comes with a necessary bias correction, due to the inconsistent radiative assumptions among the different models (surface, aerosols, clouds, etc.). More effort is needed to support both communities to overcome this issue, improving the consistency of the products (thus reducing the bias) or directly assimilating radiances.
<b>Clouds</b>	
<b>R30</b>	<p>The audience expressed the need to further study cloud shadow and 3D cloud effects. This should include:</p> <ul style="list-style-type: none"> <li>• For cloud shadow corrections a validated cloud shadow (fraction) product is needed. Cloud shadow effects on trace gas retrievals should be observationally verified preferably by combining satellite- and ground-based measurements.</li> <li>• The impact of 3D cloud shape and cloud shadow on cloud retrievals;</li> <li>• The 3D cloud effects on aerosol retrievals close to clouds edges;</li> <li>• Cloud shadow impacts on CO<sub>2</sub> and CH<sub>4</sub> may be important and mitigation methods are needed for accurate measurements of anthropogenic emissions.</li> </ul>
<b>R31</b>	The audience highlighted the importance of cloud height knowledge. The choice of cloud retrieval algorithm can have a considerable impact on trace gas retrievals, e.g., where a change of algorithm version number can lead to noticeable differences. Work on cloud retrieval algorithms deserves to be studied further.
<b>R32</b>	There is still some discrepancy between cloud products in the polar regions over land and ocean for many satellite instruments and it is important to consider vertical structure and mixed phase cloud. More needs to be invested in this respect.
<b>R33</b>	There are some new products in extracting cloud microphysics from the IR spectral domain. This has a potential to be studied further specifically in polar regions in winter.



<b>R34</b>	Spectral line databases (e.g. HITRAN) and water vapour continuum representations appear to generally be improving agreement between model and observations. More observations and further spectroscopic database improvements are required though.
<b>Terrestrial Products</b>	
<b>R35</b>	A request for the continued generation of SIF products from hyperspectral instruments (as demonstrated for e.g. Sentinel-5P) and also for future missions has been expressed. This should also include an effort on instrument intercalibration.
<b>Calibration and Validation</b>	
<b>R36</b>	On Cal/Val the audience requested support for ground-based observations that are crucial for any satellite product comparison activities. The following aspects should be addressed: <ul style="list-style-type: none"> <li>• Make use of trans-national research infrastructures and data sets for multiple Cal/Val projects or campaigns. Foster collaboration across organisations to access facilities (mobile instrumentation and fixed observatories) and co-design activities such as measurements campaigns and training;</li> <li>• Coordinate between different ground-based networks to report uncertainties in a similar way, considering both random and systematic values;</li> <li>• Harmonise reference datasets from networks such as TCCON and MUSICA-NDACC;</li> <li>• Further advanced platforms that provide access to diverse data and advanced possibilities for using and visualising data in Cal/Val activities.</li> </ul>
<b>R37</b>	ESA shall continue to play an active role in Cal/Val activities for atmospheric Sentinels (Sentinel-4, Sentinel-5, CO2M) to support campaigns to maximise the scientific use of those missions.
<b>R38</b>	ESA to initiate and support (airborne) campaigns in relation to emission quantification on different scales verifying/validating related satellite derived emission products, as emissions will become one of the most important products from atmospheric EO in air pollution as well as for greenhouse gases. In this context the knowledge of the wind field is one of the most important input parameters (and source of errors). It is recommended that ESA initiates a measurement campaign with combined trace gas imager and wind LIDAR on ideally one aircraft.
<b>Earth Explorers</b>	
<b>R39</b>	When developing new data products for ESA Earth Explorers, a close link to the DISC teams is recommended to further maximise expert input/feedback on data processing, quality and measurement information content.
<b>R40</b>	A monthly-mean L2A product (L3) should be developed from Aeolus retrievals. This product should be compared to CALIPSO L3 to examine possible biases. A homogenization process should be developed and applied before comparison.
<b>R41</b>	Through the synergy of L2A and L2B products, Aeolus provides the means to understand the properties and lifetime of smoke particles in the stratosphere, as well as their impact on dynamics and climate. A study mobilising expertise in Aeolus observations, state-of-the-art ground-based

	LIDAR microphysical retrievals, atmospheric radiative transfer, and comprehensive global climate modelling, could provide a complete assessment on the multifaceted climatic relevance of stratospheric smoke.
<b>Missions and Concepts</b>	
<b>R42</b>	<p>Beyond the already planned European missions, the audience raised the strategic need for an adequate capability of space-based limb sounding of atmospheric composition from the upper troposphere to the lower thermosphere. This is part of a wider discussion of the needs for a strategic European component in atmospheric composition monitoring as a key part of the research in environmental and climate change. In more detail, a strengthening of a continuous limb observation program is essential for:</p> <ul style="list-style-type: none"> <li>• Tropospheric ozone from limb-nadir matching;</li> <li>• Ozone-climate interaction and ozone recovery (e.g. NO<sub>y</sub>, HO<sub>y</sub>, BrO<sub>y</sub>, O<sub>x</sub>);</li> <li>• Monitoring upper atmospheric circulation in response to climate change (passive tracers: e.g. CO, N<sub>2</sub>O, CH<sub>4</sub>);</li> <li>• Long-term weather forecast (impact of stratosphere on tropospheric weather);</li> <li>• Stratosphere-troposphere exchange/UTLS (climate sensitive region);</li> <li>• Stratospheric aerosols, i.e. impact of major/minor volcanic eruptions and pyro-fire events on climate;</li> <li>• A redundancy of observations and a combination of observations in different spectral ranges (UV, Vis, IR, MW) is of great advantage.</li> </ul>
<b>R43</b>	<p>ESA should increase its attention to commercial remote sensing, especially to the so-called “New Space” observations, which have been gradually appearing over recent years. These observations may be a highly valuable addition to conventional Earth Science observations by ESA and other space agencies. Such observations may complement spatial coverage and temporal records of overall Earth observation and significantly help the scientific community to further advance research. Commercial observations can also be used for testing various observational and processing aspects in preparation of ESA’s future missions. Therefore, ESA shall encourage the development of the private Earth Observation sector and markets by investing into the on-boarding of private instruments in ESA missions, integrating small and medium satellite observations produced by the private sector into the overall data provision. Beyond that ESA shall develop a landscape that allows for maturing commercial satellite observations and reaching the quality standards of mainstream space observations.</p>