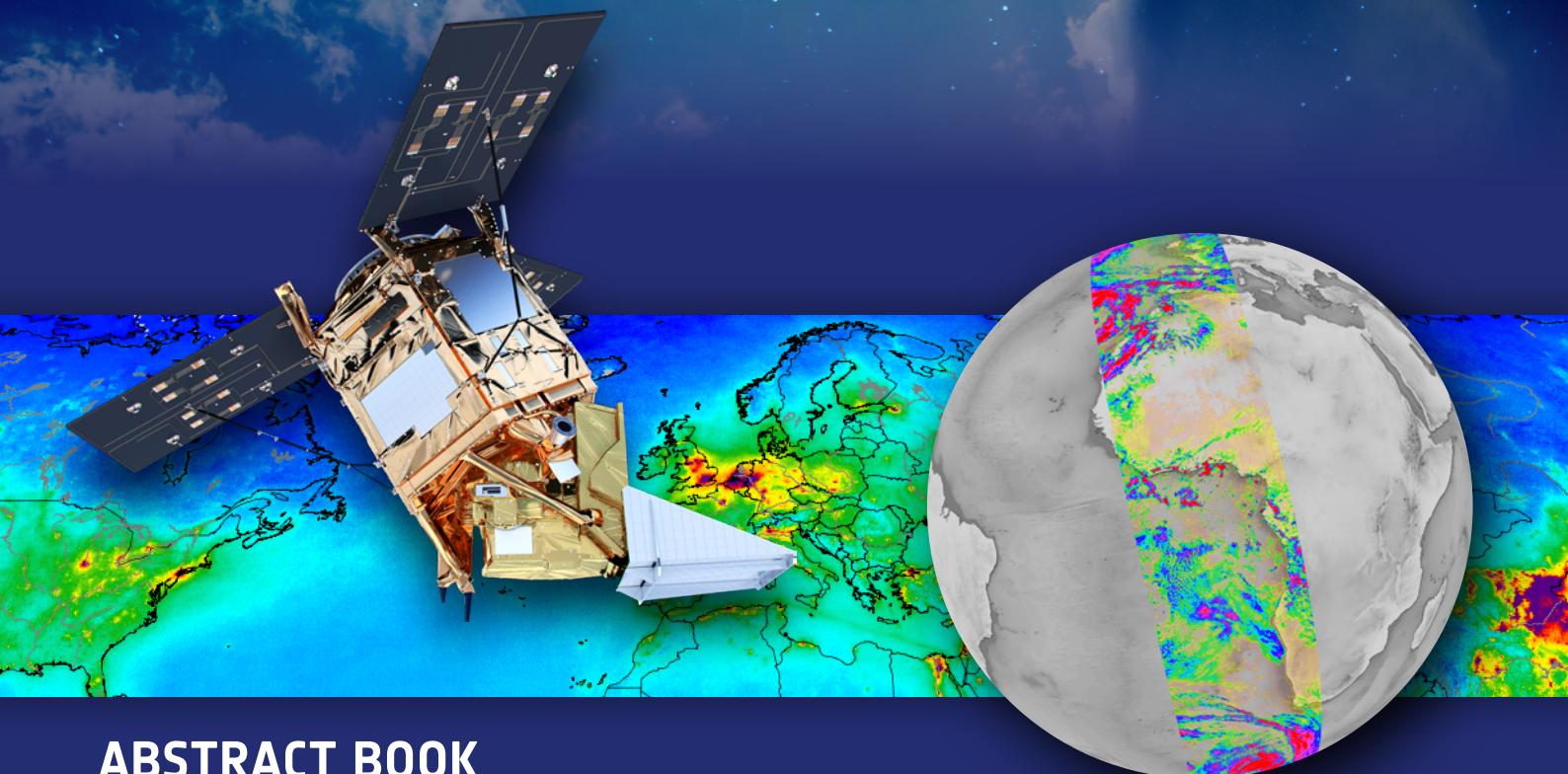




European Union



# → COPERNICUS SENTINEL-5 PRECURSOR VALIDATION TEAM WORKSHOP



## ABSTRACT BOOK

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## 2. Committees

### Scientific Committee

- Claus Zehner – ESA – Italy
- Vitali Fioletov – Environment Canada - Canada
- Norman T. O'Neill – University Sherbrooke – Canada
- Jean-Christopher Lambert – BIRA/IASB - Belgium
- Diego Loyola – DLR – Germany
- Hiroshi Suto – JAXA - Japan
- Pepijn Veefkind – KNMI – The Netherlands
- Ilse Aben – SRON – The Netherlands
- Hartmut Boesch – University Leicester - UK
- Shobha Kondragunta – NOAA - USA
- Nickolay Krotkov – NASA - USA
- Kelly Chance - Harvard-Smithsonian Center for Astrophysics - USA



### 3. Abstracts

#### Opening

##### Status of the Sentinel-5 Precursor Mission

*Dr. Claus Zehner<sup>1</sup>*

<sup>1</sup>ESA

The Sentinel-5 Precursor mission, launched on Oct. 13 2017, is the first atmospheric Sentinel and supports Copernicus services in particular for atmospheric applications, including activities such as air quality, ozone and climate monitoring. The instrument TROPOMI (Tropospheric Monitoring Instrument) is the single payload of the Sentinel-5 Precursor satellite and was co-funded by ESA and The Netherlands. Sentinel-5 Precursor ensures on the one hand continuity of atmospheric satellite data provision from the ESA ERS (GOME), ENVISAT (SCIAMACHY), and the USA EOS-AURA (OMI) missions in the various application and scientific domains and prepares on the other hand for the future atmospheric Copernicus Sentinel-4 and Sentinel-5 instruments hosted on EUMETSAT platforms. Key features of the TROPOMI instrument are global coverage within one day and providing a spatial resolution of 7.2 x 3.6 km and since August 06 2019 of 5.6 x 3.6 km. The Sentinel-5 Precursor mission has successfully finalised the Commissioning Phase on April 24 2018 and all products except ozone profiles are being provided to the user community via the Copernicus Data Hub – s5phub.copernicus.eu. This presentation provides an overview about the Sentinel-5 Precursor Mission status.

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#### Level 1

##### Tracking TROPOMI (Bands 1-6) performance with solar (V1) irradiances

*Dr. Sergey Marchenko<sup>1,2,3</sup>, Dr. Matthew DeLand<sup>1,2,3</sup>*

<sup>1</sup>Science Systems and Applications, Inc., <sup>2</sup>NASA

*Goddard Space Flight Center, <sup>3</sup>S5PVT support team-member (NASA/GSFC)*

Solar irradiance measurements from TROPOMI can provide valuable information about both instrument performance and solar variability related to climate forcing. Using the high-quality solar data produced by Aura OMI as a reference, we characterize TROPOMI performance in Bands 1-6, specifically addressing the metrics relevant to trace-gas retrievals: the instrument spectral response function, the additive components, the spectral aging, among others.

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## Campaigns

### Overview of the TROPOMI Validation Experiment in The Netherlands

*Mr Arnoud Apituley<sup>1</sup>, Dr Karin Kreher<sup>9</sup>, Dr. Ankie Piters<sup>1</sup>, Dr Tim Vlemmix<sup>1</sup>, Dr John Sullivan<sup>4</sup>, Dr Tom McGee<sup>4</sup>, Ms Mirjam Den Hoed<sup>1</sup>, Dr Bas Henzing<sup>11</sup>, Mr Arnoud Frumau<sup>11</sup>, Dr Pepijn Veefkind<sup>1</sup>, Prof.dr. Alkis Bais<sup>12</sup>, Dr. Elena Spinei Lind<sup>8</sup>, Dr. Steffen Dörner<sup>3</sup>, Dr Michel van Roozendael<sup>2</sup>, Dr Alexis Merlaud<sup>2</sup>, Dr Eduardo Landulfo<sup>5</sup>, Mr Dimitris Karagkiozidis<sup>12</sup>, Dr Diego Alves Gouveia<sup>7</sup>, Dr Alexandre Cacheffo<sup>6</sup>, Mr. Bart Speet<sup>11</sup>, Dr Richard Querel<sup>10</sup>, Dr Alex Mendes<sup>7</sup>, Dr Fabio Lopes<sup>7</sup>*

<sup>1</sup>KNMI, <sup>2</sup>BIRA, <sup>3</sup>MPIC, <sup>4</sup>NASA-GSFC, <sup>5</sup>IPEN, <sup>6</sup>UFU, <sup>7</sup>IFUSP, <sup>8</sup>Virginia Tech, <sup>9</sup>BKS, <sup>10</sup>NIWA, <sup>11</sup>TNO, <sup>12</sup>AUTH

A Sentinel-5p/TROPOMI validation campaign was held in the Netherlands based at the Cabauw Experimental Site for Atmospheric Research during September 2019. The TROpomi vaLidation eXperiment (TROLIX) consisted of active and passive remote sensing platforms in conjunction with several balloon-borne, airborne and surface atmospheric composition measurements. The goal of this geophysical validation campaign was to make intensive observations to establish the quality of TROPOMI L2 main data products (UVAI, Aerosol Layer Height, NO<sub>2</sub>, O<sub>3</sub>, HCHO, Clouds) under realistic, non-idealized circumstances with varying cloud cover and a wide range of atmospheric conditions.

Since TROPOMI is a hyperspectral imager with a very high spatial resolution of 3.6x5.6 km<sup>2</sup>, understanding local effects such as inhomogeneous sources of pollution, sub-pixel clouds and variations in ground albedo is important to interpret TROPOMI results. Therefore, the campaign includes sub-pixel resolution local networks of sensors, involving Pandora and MAXDOAS instruments, around Cabauw (51.97° N, 4.93° E) and within the city of Rotterdam. Cabauw is considered rural while Rotterdam is densely populated and industrialized.

Cabauw, using its comprehensive in-situ and remote sensing observation program in and around the 213 m meteorological tower, was the main site of the campaign with focus on vertical profiling using lidar instruments for aerosols, clouds, water vapour,

tropospheric and stratospheric ozone, as well as balloon-borne sensors for NO<sub>2</sub> and ozone.

The data set collected can be directly compared to the TROPOMI L2 data products, while measurements of parameters related to a-priori data and auxiliary parameters that influence the quality of the L2 products such as aerosol and cloud profiles and in-situ aerosol and atmospheric chemistry were also be collected.

The campaign was be supported by satellite observations and atmospheric modelling (CAMS).

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### Overview and calibration/validation plans of the Geostationary Environment Monitoring Spectrometer (GEMS)

*Ms. Hae-Jung Lee<sup>1</sup>, Mr. Jong-Min Yoon<sup>1</sup>, Mr. Limseok Chang<sup>1</sup>, Mr. Hyunkee Hong<sup>1</sup>, Mr. Won Jun Choi<sup>1</sup>, Mr. Chang Suk Lee<sup>1</sup>, Mr. Dong-Won Lee<sup>1</sup>*

<sup>1</sup>Environmental Satellite Center, National Institute of Environmental Research

The Geostationary Environment Monitoring Spectrometer (GEMS), scheduled to be launched in March 2020, will become the first space-based instrument to observe air quality from geostationary orbit. Main products of GEMS include O<sub>3</sub>, aerosol, and their precursors (e.g. NO<sub>2</sub>, SO<sub>2</sub>, HCHO, and CHOCHO) in column density. These products will mainly be used to support monitoring and forecasting of air quality and short-lived climate pollutants over East Asia. The L2 retrieval algorithms for GEMS were developed and their performance has been evaluated using synthetic radiance and L1B radiance data acquired by the Ozone Monitoring Instrument (OMI) and the Tropospheric Monitoring Instrument (TROPOMI). The Environmental Satellite Center (ESC) of the National Institute of Environmental Research (NIER) in Korea has plans to calibrate and validate the products retrieved from GEMS after launch. First is the Announcement of Opportunity (AO) for GEMS calibration and validation. The AO White Paper is being developed and expected to be completed by January 2020. The AO call will open from January to February 2020 and the relevant activities will start in March 2020. Second, an intensive campaign is planned. In 2016, NIER carried out the Korea US Air Quality (KORUS-AQ) campaign with NASA and there has been need for a follow-up campaign. While KORUS-AQ focused on the Korean peninsula, the second campaign is expected to extend its coverage to the GEMS domain and attract more researchers from various countries. One of the main proposes of this

campaign is to calibrate and validate GEMS products using ground-based (e.g. Pandora, Multi Axis-DOAS, Sunphotometer, etc.) and airborne (e.g. GEOCAPE Airborne Simulator or Geostationary Trace gas and Aerosol Sensor Optimization) instruments. A pre-campaign is also planned (2020-2021) prior to the second international campaign scheduled for 2022-2023.

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in climate tailored reprocessings as part of CCI/C3S activities. We also introduce the algorithmic updates that have been recently implemented within the TROPOMI L2 processor V2. For example, one major update in the NRTI product is the use of the dynamical TROPOMI Geometry-dependent Effective Lambertian Equivalent Reflectivity (GE\_LER) data instead of the OMI LER climatology for prescribing the scene brightness in the AMF computation.

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### TROPOMI/S5P near-real time and offline total ozone column products

*Christophe Lerot<sup>1</sup>, Klaus-Peter Heue<sup>2</sup>, Fabian Romahn<sup>2</sup>, Jian Xu<sup>2</sup>, Walter Zimmer<sup>2</sup>, Diego Loyola<sup>2</sup>, Michel Van Roozendael<sup>1</sup>, Tijl Verhoevel<sup>1</sup>, Katerina Garane<sup>3</sup>, MariLiza Koukouli<sup>3</sup>, Dimitris Balis<sup>3</sup>, Jean-Christopher Lambert<sup>1</sup>*

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The near-real time (NRTI) and offline (OFFL) total ozone columns are derived from TROPOMI/S5p radiance measurements using two different retrieval algorithms. On one hand, ozone columns are produced with the DOAS-type GDP algorithm, which follows the requirements of a near-real time processing. On the other hand, the offline product is based on the direct-fitting algorithm GODFITv4 in order to ensure consistency with long-term total ozone Climate Data Records (CDR), since this algorithm has been applied to heritage and current instruments (GOME, SCIAMACHY, GOME-2, OMI and OMPS) as part of ESA CCI and Copernicus C3S activities.

We present briefly the two TROPOMI total ozone column products, their status and how they intercompare with each other. We also assess their level of mutual consistency with other satellite L2 data sets as produced either in operational environments or

### First Total Ozone Column validation results of TRO3VALAG project

*Dr. John Christodoulakis<sup>1</sup>, Mr. Georgios Kouremadas<sup>1</sup>, Mrs. Eleni Fotini Fotaki<sup>1</sup>, Prof. Costas Varotsos<sup>1</sup>*

<sup>1</sup>National & Kapodistrian University Of Athens

The validation of the daily observations of the Total Ozone Column (TOC) obtained by the TROpospheric Monitoring Instrument (TROPOMI), and the Dobson spectrophotometer No. 118 located at Athens, Greece, (WOUDC Station ID: 293) during the period 1/Nov/2017 – 31/Oct/2019 is attempted here. For validation purposes, the previous sensing period is divided into two parts. First part, from 1/Nov/2017 to 21/Aug/2019, covers the initial validation period. The analysis performed during this period is based on the use of satellite observations located at distances from a ground-based station of less than 100 km and within a 2 hour time frame. Among others, this analysis attempts to answer the question that is being raised during satellite validation efforts “Should the nearest spatial or temporal satellite observation be compared with the ground-based?”.

Since 22/Aug/2019, we have available simultaneous ground-based and satellite observations. In addition to studying the TOC differences between the satellite observations closest to the ground-based (spatial and temporal), we make a first attempt to perform a spatial analysis of the observed differences in an area 500 km around ground-based station. The objective is to study the spatial comparability of a ground-based Dobson station (in this case the Athens station) in satellite observations obtained within this limit.

For all the aforementioned analyses, Near-Real-Time, Offline and Reprocessed dates have been used depending on their availability.

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## **TROPOMI S5P total ozone column global validation within the VALTOZ project**

*Dr. Katerina Garane<sup>1</sup>, Dr. Maria-Elissavet Koukouli<sup>1</sup>, Ms. Fani Gkertsis<sup>1</sup>, Dr. Christophe Lerot<sup>2</sup>, Dr. Klaus-Peter Heue<sup>3</sup>, Dr. Tijl Verhoelst<sup>2</sup>, Prof. Dimitris Balis<sup>1</sup>, Dr. Vitali Fioletov<sup>4</sup>, Dr. Alberto Redondas<sup>5</sup>, Dr. Fabian Romahn<sup>3</sup>, Dr. Walter Zimmer<sup>3</sup>, Dr. Andrea Pazmino<sup>6</sup>, Dr. Ariane Bazureau<sup>6</sup>, Prof. Alkiviadis Bais<sup>1</sup>, Dr. Jean-Christopher Lambert<sup>2</sup>, Dr. Diego Loyola<sup>3</sup>, Dr. Michel Van Roozendael<sup>2</sup>, Dr. Florence Goutail<sup>6</sup>, Dr. Jean-Pierre Pommereau<sup>6</sup>, Prof. Christos Zerefos<sup>7</sup>*  
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The Laboratory of Atmospheric Physics of the Aristotle University of Thessaloniki, Greece, is the co-ordinator of the Validation of S5P/TROPOMI total ozone, VALTOZ, team. The S5P/TROPOMI total ozone validation is performed on a global scale using Brewer, Dobson and UV-visible/SAOZ networks. In this work the TROPOMI Near-Real Time, NRTI, and Offline, OFFL, total ozone column (TOC) products are presented and compared to globally distributed and quality-assured daily ground-based Brewer and Dobson TOC measurements, deposited in the World Ozone and Ultraviolet Radiation Data Centre (WOUDC). The quality of the TROPOMI TOC data is evaluated in terms of the effect of many influence quantities, such as solar zenith angle, clouds, surface albedo, etc. The mean bias and the mean standard deviation that results from the comparisons is also evaluated against the S5P product requirements. Moreover, other well-established space-borne sensors (e.g. OMPS/ Suomi-NPP, GOME-2/MetopA and GOME-2/MetopB) are utilized to further assess the TROPOMI OFFL and NRTI products quality.

Additional comparisons to individual Brewer measurements from the Canadian Brewer Network and the European Brewer Network (Eubrewnet), as well as MAX-DOAS instruments, are also performed to examine how the diurnal variation of TOC is captured by S5P/TROPOMI.

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## **Global validation of S5P OFFL V1.05/1.07 total ozone by comparisons with S5P IUP-WFDOAS V4 total ozone**

*Mark Weber<sup>1</sup>, Kai-Uwe Eichmann<sup>1</sup>*

*<sup>1</sup>University of Bremen FB1*

The S5P/TROPOMI operational offline total ozone in its data versions 1.05/1.07 will be compared with the scientific TROPOMI WFDOAS V4 total ozone that has been retrieved at IUP Bremen. The WFDOAS V4 total ozone is based upon the weighting function DOAS approach that has been successfully applied to GOME, SCIAMACHY and GOME-2 aboard the three Metop satellites A to C. The WFDOAS algorithm in its newest version (V4) uses the following settings: Serdyuchenko ozone absorption cross-sections corrected for the lo-effect, LUT-based polarisation correction and Ring pseudo-absorber spectra. Adaptation of auxiliary input spectra to the spectral resolution of the instrument is done on-the fly (one algorithm for all satellite instruments). The WFDOAS algorithm is quite similar to the GODFIT algorithm used in the operational retrieval as both embed a radiation-transfer module in their retrieval scheme.

In this talk the side-to-side validation of both ozone data products (OFFL and WFDOAS) by comparisons with Brewer and Dobson ground data will be presented as well as direct global comparisons between both algorithms for the time frame November 2017 until September 2019 shown. Initial results show that WFDOAS V4 total ozone shows very good precision with respect to ground data (within 1.5% at 1sigma for most Brewer stations) and no drifts during the early mission period. The overall bias with respect to ground strongly depends on the ozone absorption cross-section used in the retrieval and may vary by up to 3%.

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## **Operational validation of Sentinel-5p TROPOMI near-real time and offline total ozone column products**

*Dr. Tijl Verhoelst<sup>1</sup>, Katerina Garane<sup>2</sup>, Jean-Christopher Lambert<sup>1</sup>, Sander Niemeijer<sup>5</sup>, Maria-Elissavet Koukouli<sup>2</sup>, Dimitris Balis<sup>2</sup>, Christophe Lerot<sup>1</sup>, Michel Van Roozendael<sup>1</sup>, Klaus-Peter Heue<sup>3</sup>, Diego Loyola<sup>3</sup>, Jose Granville<sup>1</sup>, Andrea Pazmino<sup>4</sup>, Florence Goutail<sup>4</sup>, Jean-Pierre Pommereau<sup>4</sup>*

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In this contribution we summarize one and half year of ground-based validation for both the Sentinel-5p TROPOMI NRTI and OFFL total O<sub>3</sub> (L2\_O<sub>3</sub>) products, carried out by the operational validation service of the Sentinel-5p Mission Performance Centre (MPC), using independently the MPC Automated Validation Server (VDAF-AVS) and the satellite validation systems at BIRA-IASB (Multi-TASTE) and AUTH. Those three validation systems perform comparisons to complementary types of ground-based measurements collected from worldwide monitoring networks archiving regularly data into the NDACC and WOUDC databases, i.e. direct-sun observations with Brewer and Dobson UV spectrophotometers, and twilight zenith-sky observations with ZSL-DOAS UV-visible instruments (and particularly the NDACC SAOZ network with its near-real-time processing facility). Altogether, the complementary networks provide deep insight into satellite ozone data quality with wide geographical coverage, regular sampling of meridian structures and seasonal cycles, and validation under the most difficult observing conditions like low sun elevation, high cloudiness, and complex surface albedo like sea/ice. Particular attention is paid to new developments since the last S5PVT workshop, such as the TROPOMI switch to smaller ground pixel size in August 2019 and the upcoming update of the TROPOMI Level-2 data processors to V2, evaluated here using a diagnostic data set (DDS). A first evaluation of the ex-ante uncertainties provided by the TROPOMI product developers is attempted, as this is a specific theme for the workshop. We conclude with a brief survey of validation and evaluation results from different AO projects, satellite-to-satellite intercomparisons, data assimilation studies performed by the Copernicus Atmosphere Monitoring Service at ECMWF (CAMS), and the literature.

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## Tropospheric Ozone

**TROPOMI S5P tropospheric ozone columns data retrieval and validation**

*Klaus-Peter Heue<sup>1</sup>, Diego Loyola<sup>1</sup>, Fabian Romahn<sup>1</sup>, Daan Hubert<sup>2</sup>, Tijl Verhoelst<sup>2</sup>, Arno Keppens<sup>2</sup>, Christophe Lerot<sup>2</sup>*  
<sup>1</sup>DLR, <sup>2</sup>BIRA / IASB

Based on the OFFL total ozone columns and the cloud data the tropical tropospheric ozone columns are calculated with the convective cloud differential (CCD) method. This algorithm implies the stratospheric column to be constant in time for a few days at least and longitudinal constant. Both requirements are fulfilled in the tropical band between 20° South and 20° North.

The tropical tropospheric ozone columns are gridded to a 0.5° latitude x 1° longitude grid. They encompass a time period for 5 days for the stratosphere and 3 days for the tropical troposphere. Since December 2018 the data are operationally available.

We present the algorithm and the latest updates. The data are regularly compared to similar data from other satellite missions (GOME-2B and OMI).

In the framework of the S5P MPC the tropospheric ozone columns are validated against integrated ozone sondes. The sonde data are available via the SHADOZ network as well as WOUDC (World Ozone and Ultraviolet Radiation Data Centre). For the individual sonde station the mean bias and standard deviations are also compared to the user requirements.

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### Assessment of Sentinel-5p Tropospheric Ozone using SHADOZ Ozonesonde Network Data

*Daan Hubert<sup>4</sup>, Arno Keppens<sup>1</sup>, Tijl Verhoelst<sup>1</sup>, Steven Compernolle<sup>1</sup>, José Granville<sup>1</sup>, Jean--Christopher Lambert<sup>1</sup>, Klaus-Peter Heue<sup>2</sup>, Diego Loyola<sup>2</sup>, Kai-Uwe Eichmann<sup>3</sup>, Mark Weber<sup>3</sup>, Marc Allaart<sup>4</sup>, Ankie Piters<sup>4</sup>, Anne Thompson<sup>5</sup>, Ryan Stauffer<sup>5</sup>, Debra Kollonige<sup>5,6</sup>, Bryan Johnson<sup>7</sup>, Hölder Vömel<sup>8</sup>, Henry Selkirk<sup>5,9</sup>, F da Silva<sup>10</sup>, M Mohamad<sup>11</sup>, Christian Félix<sup>12</sup>, Gérard Ancellet<sup>13</sup>, Andy Delcloo<sup>14</sup>, Valentin Duflot<sup>15</sup>, Sophie Godin-Beekmann<sup>16</sup>, Thierry Leblanc<sup>17</sup>, Wolfgang Steinbrecht<sup>18</sup>, René Stübi<sup>12</sup>*

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Tropospheric ozone is a pollutant that damages ecosystems and triggers human health issues. Ozone concentrations are highly variable over time and across the troposphere, which poses clear challenges to deepen our understanding of the processes involved in the production and transport of ozone. Further progress depends on the availability of instruments capable of measuring tropospheric ozone and its distribution at finer spatio-temporal scales. The TROPOMI instrument on the Sentinel-5p platform, launched in October 2017, combines a high spatial resolution, a large swath width and the spectral measurement characteristics required to deliver tropospheric ozone data records at unprecedented detail. The first of these products was released in fall 2018. It consists in  $0.5^{\circ}$  (latitude) by  $1^{\circ}$  (longitude) resolved daily maps of 3-day moving mean values of the tropospheric ozone column between  $20^{\circ}\text{S}$  and  $20^{\circ}\text{N}$ , computed using the convective-cloud method (CCD). Two other tropospheric data products (upper tropospheric mixing ratios by the Cloud Slicing Algorithm (CSA) and vertically resolved tropospheric ozone by an Optimal Estimation retrieval scheme) are still being fine-tuned and will be released in the near future.

We present an assessment of the quality of the Sentinel-5p TROPOMI convective-cloud tropospheric ozone column data carried out within the context of ESA's Sentinel-5p Mission Performance Centre (MPC) and the S5PVT AO project CHEOPS-5p (Validation of Copernicus Height-resolved Ozone data Products from Sentinel-5p TROPOMI using global sonde and lidar networks, #28587). The studied TROPOMI data (L2\_O3\_TCL OFFL) is produced operationally by the OFFL processor (v01.01.05-01.01.07). We show how routine visual inspections of the tropospheric ozone fields uncover non-geophysical structures like geographical stripes. These are introduced by the sampling pattern of the instrument and possibly also by a dependence of the quality of Sentinel-5p retrieved total ozone data on cloud parameters. The assessment of TROPOMI data quality is furthermore based on comparisons to co-located quality-assured ozonesonde measurements associated with the SHADOZ network. This well-characterized observational data record serves as a reference to evaluate the bias and other uncertainty estimates of the Sentinel-5p data, and their dependence on influence quantities. Our study concludes with a verification of the compliance of Sentinel-5p tropospheric ozone data with respect to mission and user requirements for key data applications.

## S5p/TROPOMI tropical tropospheric ozone: verification of the CCD operational algorithm L2\_O3\_TCL and advances of the CSA prototype

*Mark Weber<sup>1</sup>, Kai-Uwe Eichmann<sup>1</sup>, Elpida Leventidou<sup>1</sup>, Klaus-Peter Heue<sup>2</sup>*

<sup>1</sup>*University of Bremen FB1*

This talk covers the two algorithms to retrieve tropospheric ozone in the tropics. The convective cloud differential method (CCD) is already operational. We compare the L2\_O3\_TCL version 01.01.05 with CCD algorithm results, using S5p WFDOAS v4 total ozone and L2\_CLOUD data.

The cloud slicing algorithm (CSA) has now been improved to better cope with the spatially high resolution data of S5p and is ready for implementation into the operational processor. Results using S5p L2 V01.01.07 data will be presented and first validation using SHADOZ V6 ozone sonde will be presented.

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## Aerosol Information

### Aerosol Index: overview of intercomparison results and future updates

*Dr. Deborah Stein Zweers<sup>1</sup>, Dr. Thomas Wagner<sup>2</sup>, Dr. Maarten Sneep<sup>1</sup>, Dr. Piet Stammes<sup>1</sup>, Dr. Gijsbert Tilstra<sup>1</sup>, Dr. Omar Torres<sup>3</sup>*

<sup>1</sup>*KNMI - Royal Netherlands Meteorological Institute,*

<sup>2</sup>*Max Planck Institute for Chemistry, <sup>3</sup>NASA Goddard Space Flight Center*

Aerosol Index (UVAI) data from TROPOMI on board Sentinel 5-P has been verified and validated using satellite-to-satellite intercomparisons with other instruments including the Ozone Mapping and Profiler Suite (OMPS) and Ozone Monitoring Instrument (OMI). Several examples show that structures are well captured for typical sources of UV-absorbing aerosols including volcanic ash, desert dust, and smoke from biomass burning. It is known that the UVAI is very sensitive to absolute radiance. Therefore, monitoring the global mean and median is a good indicator of the state of the calibration of L1b data. Information about the impacts of the known wavelength-dependent degradation on UVAI will be presented as well as how this will be taken into account with the next L1b 2.0.0 update. Finally, a brief outlook will be given regarding future updates to the TROPOMI UVAI data product including possible approaches to address the effect of cloud and cloud structures on the aerosol index.

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### S5P/TROPOMI Aerosol Layer Height Product validation and recent improvements

*Dr. Martin De Graaf<sup>4</sup>, Mr. Swadwin Nanda<sup>1</sup>, Dr. Maarten Sneep<sup>1</sup>, Mr. Mark ter Linden<sup>2</sup>, Dr. Pepijn Veefkind<sup>1</sup>*

<sup>1</sup>*KNMI, <sup>2</sup>S&T*

The S5P/TROPOMI Aerosol Layer Height (ALH) L2 product was recently released to the public (30 Sept. 2019), after intense development to make the product suitable for near-real time (NRT) processing of global data. The TROPOMI ALH product is the first product that provides aerosol height information with global

coverage. It is derived from the O2-A band measured by TROPOMI in cloud-free scenes with sufficient aerosol loading. In this presentation, the most recent developments will be summarized, and the first validation efforts of the new product will be presented. The ALH product shows a close correlation with CALIOP weighted mean extinction height for scenes that are strictly cloud-free, with an underestimation of the ALH of about 500 m compared to CALIOP weighted mean extinction height that may be attributed to different sensitivities of the derived heights. The TROPOMI ALH shows good correlation with MISR plume height retrievals and ground-based lidar measurements, but these validation results have to be further extended. The main remaining issues for the ALH are a proper screening of clouds, which is essential for the correct retrieval of the aerosol layer height, surface albedo effects that bias the retrieval especially for bright surfaces, and the selection criteria for scenes with sufficient aerosol loading. The presentation will briefly touch on the next developments steps for the algorithm and the outlook for the TROPOMI ALH product.

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### Validation of UV Aerosol Index and Aerosol Layer Height Product from S5P TROPOMI

*Dr. Pubu Ciren<sup>1</sup>, Dr. Shobha Kondragunta<sup>2</sup>*

<sup>1</sup>*IMSG Inc. & NOAA/NESDIS/STAR,*

<sup>2</sup>*NOAA/NESDIS/STAR*

The NOAA proposed activities to European Space Agency (ESA) for Sentinel 5 Precursor Tropospheric Ozone Monitoring Instrument (S5P TROPOMI) calibration/validation activities include exploring the possibility of a synergistic retrieval using measurements from VIIRS and TROPOMI to improve the accuracy of VIIRS ADP. As a first step of these proposed activities, we validated both UV AAI and Aerosol Layer Height product from S5P TROPOMI by comparisons with AAI from NOAA VIIRS ADP and Vertical Feature Mask from CALIOP for the time period from May, 2018 to October, 2019. It includes both biomass burning events in the United States and Canada and several dust events. Early analyses indicate that TROPOMI UV AAI has an advantage of identifying aerosols over clouds and bright surface while the VIIRS has an added ability of separating smoke from dust. However, TROPOMI AAI values have a low bias and thus not detecting the full extent of smoke plume correctly. The plume height from TROPOMI aerosol layer height (ALH) product, in general, agrees with aerosol/cloud layer height from CALIOP. Its coverage is dependent on TROPOMI AAI. In this presentation, we will report our findings through

full statistical analysis of about one and half year of CALIOP VFM and TROPOMI AAI/ALH with results stratified for dust, smoke, and haze. In addition, results from cases studies, including both local and transported smoke/dust events, will be also presented.

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### Ozone Validation activities at ALOMAR and Sodankylä

*Ms. Malin Abrahamsen<sup>1</sup>, Dr.rer.nat. Michael Gausa<sup>1</sup>, Dr. Rigel Kivi<sup>2</sup>, Ms. Ingrid Hanssen<sup>1</sup>*

<sup>1</sup>*Andøya Space Center, <sup>2</sup>Finish Meteorological Institute*  
The Arctic Lidar Observatory for Middle Atmosphere Research (ALOMAR) at Andøya Space Center is participating in the validation of Tropomi products with a number of instruments, and we will be presenting results from several of these. The location at 69N, 16E is distinguished by a high number of overpasses, and the high latitude provides a unique perspective on several issues which might affect the data products, such as large variability of the surface albedo in the Arctic, the long twilight period and a high solar zenith angle.

In cooperation with the Finish Meteorological Institute (FMI) Arctic Research Center (67N, 26E) at Sodankylä, we compare total ozone column data from Brewer with the L2 total ozone column product for the past year. Potential issues concerning the low qa\_value for high latitudes, such as snow cover has been considered, as well as the data coverage during the extended periods of twilight during winter.

Data from the ALOMAR Ozone DIAL lidar will be used to validate the O3 profile product. The ozone lidar is capable of retrieving the ozone density and ambient temperature in a height range of 9 to 50 km. The co-located ALOMAR tropospheric lidar is being used to validate aerosol and cloud layer heights, and we will present different cases and compare the results with the L2 AER\_LH product.

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### Investigating the vertical and horizontal distribution of trace gases and aerosols with the 4-Azimuth-MAX-DOAS in Mainz, Germany

*Ms. Julia Remmers<sup>1</sup>, Mr. Steffen Beirle<sup>1</sup>, Mr. Sebastian Donner<sup>1</sup>, Mr. Thomas Wagner<sup>1</sup>*

<sup>1</sup>*Max Planck Institute For Chemistry*

MAX-DOAS measurements are mainly used to retrieve vertical profiles of aerosols and trace gases in the lower troposphere. Mostly it is ignored, that due to the measurement principle, these observations are

sensitive for (or affected by) horizontal inhomogeneity, too. The horizontal sensitivity range varies between 3 and 30 km, highly depending on wavelength and atmospheric conditions.

With our 4-Azimuth-MAXDOAS we perform elevation scans in four azimuth directions simultaneously. By combining all measurements, it is possible to retrieve the vertical and horizontal distribution of aerosols and trace gases and at the same time to correct for the effects of horizontal gradients.

One strength of MAX-DOAS measurements is the ability to connect satellite and local in-situ measurements, because they yield trace gas concentrations at the surface and at the same time the total tropospheric column. Therefore, we compare our results to both datasets.

To investigate the effect of the horizontal inhomogeneity on standard MAX-DOAS retrievals also a study with synthetic data was performed and will be shown.

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## Clouds

### TROPOMI/Sentinel-5 Precursor cloud products version 2 and validation

*Dr. Athina Argyrouli<sup>6,1</sup>, Dr. Ronny Lutz<sup>1</sup>, Mr. Fabian Romahn<sup>1</sup>, Dr. Diego Loyola<sup>4</sup>, Dr. Steven Compernolle<sup>2</sup>, Mr. Sander Niemeijer<sup>3</sup>, Dr. Ewan O'Connor<sup>4</sup>, Dr. Maarten Sneep<sup>5</sup>*

*<sup>1</sup>German Aerospace Center (DLR), Remote Sensing Technology Institute, <sup>2</sup>Royal Belgian Institute for Space Aeronomy (BIRA-IASB), <sup>3</sup>s[&t Corporation,*

*<sup>4</sup>Department of Meteorology, University of Reading, <sup>5</sup>Royal Netherlands Meteorological Institute (KNMI),*

*<sup>6</sup>Technical University of Munich, TUM Department of Civil, Geo and Environmental Engineering, Chair of Remote Sensing Technology*

The TROPOMI cloud retrieval is a two-step algorithm where the OCRA (Optical Cloud Recognition Algorithm) computes the cloud fraction using a broad-band UV/VIS color space approach and ROCINN (Retrieval of Cloud Information using Neural Networks) retrieves the cloud height, cloud optical thickness and cloud albedo from NIR measurements in and around the oxygen A-band (~760nm). Two cloud models are handled in ROCINN; Clouds-as-Reflecting-Boundaries (CRB) which considers the cloud as a Lambertian reflector and Clouds-as-Layers (CAL) which considers the cloud as a homogeneous cluster of scattering liquid water spherical particles using Mie theory. Several improvements have been introduced in the OCRA/ROCINN in UPAS version 02.00.01 for TROPOMI including the discrimination of the cloud phase through the temperature information at the cloud top. An additional improvement of the ROCINN cloud retrieval is achieved from the replacement of the MERIS surface albedo climatology of a coarse resolution ( $0.25^\circ \times 0.25^\circ$ ) with retrieved surface properties from TROPOMI measurements at the same NIR spectral window and updated on a daily basis. The TROPOMI surface albedo maps are much more suitable for the cloud retrieval algorithms for two reasons: terrain features, like rivers, are usually not well represented in the MERIS climatology due to the coarse resolution and, what is more important, the pixels covered by snow or ice are frequently falsely classified in the MERIS climatology. Furthermore, the OMI cloud-free composites used in OCRA have been replaced with TROPOMI cloud-free

composites resulting in a more accurate cloud fraction retrieval from TROPOMI. Finally, both the quality assurance value calculation scheme and the handling of co-registration issue between Band 3/4 and Band 6 have been improved.

Both the CAL and CRB cloud modes of the S5p CLOUD product are routinely validated within MPC. Cloud height data is obtained from the ground-based CLOUDNET network (classification profile data, provided typically each 30s and with a 50 m vertical resolution) via the EVDC portal, and this data stream is input to the MPC online automated validation server (AVS), thereby enabling automated comparisons. While these basic-level comparisons are a starting point, more advanced validation processing (adapted filter and co-location criteria) is performed to arrive at the final results.

Although the availability of CLOUDNET sites is increasing, the spatial distribution is still rather limited, dominated by European sites. Therefore, in complement, orbit-to-orbit comparisons of cloud top height and cloud optical thickness of S5p CLOUD CAL with NASA's NPP VIIRS (flying in loose formation with S5p, with <5 min temporal separation) are also performed.

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### S5P-NPP Cloud Product Status/Plans

*Mr. Richard Siddans<sup>1</sup>*

*<sup>1</sup>Stfc Ral*

This presentation will summarise the status and plans for the operational S5P-NPP Cloud product which provides information on cloud coverage for all S5P scenes derived from Suomi-NPP VIIRS data.

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### Validation of Sentinel-5p retrieved cloud height using the ground-based CLOUDNET network

*Dr. Steven Compernolle<sup>1</sup>, Dr. Athina Argyrouli<sup>2,5</sup>, Dr. Ronny Lutz<sup>2</sup>, Dr. Maarten Sneep<sup>3</sup>, Dr. Ewan O'Connor<sup>4</sup>, Dr. Jean-Christopher Lambert<sup>1</sup>*

*<sup>1</sup>Royal Belgian Institute For Space Aeronomy (BIRA-IASB), <sup>2</sup>German Aerospace Centre (DLR), Remote Sensing Technology Institute, <sup>3</sup>Royal Netherlands Meteorological Institute (KNMI), <sup>4</sup>University of*

*Reading, Department of Meteorology, <sup>5</sup>Technical University of Munich, TUM Department of Civil, Geo and Environmental Engineering*

In general, clouds can have a profound effect on satellite measurements of the tropospheric or total column of trace gas species, and this is also true for

several Sentinel-5p trace gas data products. The effect of clouds is taken into account in the S5p retrieval of trace gas data; examples are the modification of the radiative transfer and associated quantities such as the air mass factor, and the partial masking of the measurement scene. The accuracy of these corrections relies on the accuracy of the cloud properties, themselves retrieved from S5p TROPOMI data: the radiometric cloud fraction, the cloud (top) height and the cloud optical thickness/cloud albedo. For example, an error of 50 hPa in cloud pressure can lead to a 10% error in tropospheric NO<sub>2</sub> column (see S5p NO<sub>2</sub> ATBD).

Therefore, S5p cloud product validation is a part in the end-to-end validation of the following S5p data products within their corresponding AO projects: L2\_O3\_ (O<sub>3</sub> total column; project VALTOZ, #28568), L2\_O3\_TCL (O<sub>3</sub> tropospheric column; project CHEOPS-5p, #28587), L2\_HCHO\_ and L2\_NO2\_ (HCHO and NO<sub>2</sub> tropospheric column; project NIDFORVAL, #208607). These trace gas products use one of the following three S5p cloud data products : (i) OCRA/ROCINN CAL (clouds-as-layers), (ii) OCRA/ROCINN CRB (clouds-as reflecting boundaries), both of which are contained in the official S5p cloud product L2\_CLOUD\_, and (iii) the S5p support product FRESCO.

In this work, we present a validation of cloud height (S5p CLOUD CRB and S5p FRESCO) and cloud top height (S5p CLOUD CAL) S5P data using cloud profile information from the ground-based networks CLOUDNET and ARM at 13 sites. The validation approach starts from the approach by Veefkind et al. (2016) used for the evaluation of the EOS-Aura OMI O<sub>2</sub>-O<sub>2</sub> data product but is modified to suit the specifics of TROPOMI like the high horizontal resolution. Sites where the comparison is difficult (due to e.g., orography, snow/ice cover) are identified. S5P and CLOUDNET report similar cloud height variations at several sites, and the correlation between the S5p cloud products and CLOUDNET can be high (Pearson R up to 0.9). However, there is a site-dependent negative bias of the S5p cloud (top) height with respect to the CLOUDNET data: up to -2.5 km for S5p CLOUD CAL cloud top height and -1.5 km for S5p CLOUD CRB and S5p FRESCO cloud height. The dependence on other parameters measured by S5p and CLOUDNET (e.g., cloud fraction, geometrical cloud cover,...) is investigated.

## Sulfur Dioxide

### TROPOMI SO<sub>2</sub> retrievals: L2 product status, planned evolution and validation

*Dr. Nicolas Theys<sup>1</sup>, Dr Isabelle De Smedt<sup>1</sup>, Dr Christophe Lerot<sup>1</sup>, Dr Huan Yu<sup>1</sup>, Dr Jonas Vlietink Vlietink<sup>1</sup>, Dr Pascal Hedelt<sup>2</sup>, Dr Zhibin Cheng<sup>2</sup>, Dr Walter Zimmer<sup>2</sup>, Dr Fabian Rohman<sup>2</sup>, Dr Diego Loyola<sup>2</sup>, Dr Michel Van Roozendael<sup>1</sup>*

<sup>1</sup>Royal Belgian Institute For Space Aeronomy, <sup>2</sup>DLR  
BIRA-IASB and DLR have the joint responsibility of developing and maintaining the SO<sub>2</sub> retrieval algorithm and implementation into the S5P operational processor. In this presentation, we introduce the current algorithm, present the planned evolution of the product. We also show comparisons with some satellite L2 retrievals (e.g. OMI) and with correlative measurements from the ground. Validation challenges are also addressed and plans for future work are presented.

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## **Profiling Volcanic SO<sub>2</sub> with Balloonsondes in Costa Rica for TROPOMI Validation: An update**

*Dr. Henry Selkirk<sup>1,2</sup>, Dr. Nickolay Krotkov<sup>2</sup>, Dr. Gary Morris<sup>3</sup>, Dr. Pascal Hedelt<sup>4</sup>, Dr. Can Li<sup>2,5</sup>, Dr. James Flynn<sup>6</sup>*

<sup>1</sup>*Universities Space Research Association, <sup>2</sup>NASA Goddard Space Flight Center, <sup>3</sup>St. Edwards University, <sup>4</sup>German Aerospace Center, <sup>5</sup>University of Maryland College Park, <sup>6</sup>University of Houston*

Using both dual and single ozonesonde launches, the NASA/Costa Rican balloonsonde project Ticosonde has continued to monitor plumes of SO<sub>2</sub> emitted by nearby Volcán Turrialba and on at least one recent occasion, Volcán Poás. An SO<sub>2</sub> plume will cause a notch in the profile of ozone as it passes through the plume. This is caused by SO<sub>2</sub> with the redox reaction by which ozone is detected in the electrochemical concentration cell (ECC) ozonesonde. Since 2006 we have obtained over 100 ozone profiles with the telltale notches indicative of SO<sub>2</sub>. These notches are up to several kilometers in depth and are typically centered near 3.5 km, the elevation of Turrialba. Conclusive evidence of the presence of SO<sub>2</sub> in these notched profiles was obtained in early 2012 when we launched a payload with two ozonesondes which derives SO<sub>2</sub> using by simple filter differencing technique. The following year we began regularly flying these dual ozonesondes in support of OMI SO<sub>2</sub> retrieval validation. Through September 2019, we have launched 69 dual sondes, 22 of these since the launch of TROPOMI in November 2017. The data are archived at the NASA Aura Validation Data Center at [https://avdc.gsfc.nasa.gov/pub/tmp/TICOSONDE\\_SO2\\_archive/](https://avdc.gsfc.nasa.gov/pub/tmp/TICOSONDE_SO2_archive/). Here we review the SO<sub>2</sub> plumes identified in both dual and single ozone sonde launches since the TROPOMI launch. We particularly focus on how the sonde observations can be used to estimate the height and depth of the volcanic emissions plumes.

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## **Anthropogenic and volcanic point source SO<sub>2</sub> emissions derived from TROPOMI onboard Sentinel 5 Precursor: first results**

*Dr Vitali Fioletov<sup>1</sup>, Dr Chris McLinden<sup>1</sup>, Dr Debora Griffin<sup>1</sup>, Dr Nicolas Theys<sup>2</sup>, Dr Diego Loyola<sup>3</sup>, Dr Nickolay Krotkov<sup>4</sup>, Dr Can Li<sup>4,5</sup>, Dr Pascal Hedelt<sup>3</sup>, Dr Simon Carn<sup>6</sup>*

<sup>1</sup>*Environment And Climate Change Canada, <sup>2</sup>Belgian Institute for Space Aeronomy (BIRA-IASB), <sup>3</sup>Deutsches Zentrum für Luft- und Raumfahrt (DLR), <sup>4</sup>NASA Goddard Space Flight Center, <sup>5</sup>University of Maryland, <sup>6</sup>Michigan Technological University*

The paper introduces the first TROPOMI-based sulfur dioxide (SO<sub>2</sub>) emission estimates for point sources. A total of about 500 continuously emitting point sources releasing from about 10 kT y<sup>-1</sup> to more than 2000 kT y<sup>-1</sup> of SO<sub>2</sub> per year, previously identified using Ozone Monitoring Instrument (OMI) were analysed using TROPOMI measurements using data for one full year, from April 2018 to March 2019. The annual emissions from these sources were estimated and compared to similar estimates from OMI and Ozone Mapping Profiling Suite (OMPS) measurements. We were able to identify 278 sources where annual emissions are significant and can be reliably estimated from TROPOMI data. Due to its very high spatial resolution, TROPOMI produces the same number of observations monthly over a certain area as OMI produces in one year. The uncertainties of TROPOMI SO<sub>2</sub> measurements are from about 1 Dobson Unit (DU, where 1 DU = 2.69 × 10<sup>16</sup> molecules/cm<sup>2</sup>) in the tropical region to about 1.5 DU at middle and high latitudes, i.e., about 1.5 times higher than those from OMI. However due to a much larger number of pixels, annual emissions can be estimated with uncertainties that are 1.5-2 times lower than the uncertainties of annual emissions estimates from OMI. There are also systematic biases between TROPOMI and OMI over some regions, e.g., there is an about 0.5 DU bias over the Persian Gulf, that have to be removed for emission calculations.

In addition to emission estimates, direct comparisons of TROPOMI SO<sub>2</sub> with ground-based Brewer and Pandora measurements will be presented. SO<sub>2</sub> plume from the eruption of Raikoke volcano (Kuril Islands) on June 21-22 was observed over Canada in July 2019. SO<sub>2</sub> values as high as 15 DU were measured at six Brewer sites and two Pandora sites at that time.

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## **Characterization of uncertainty in the volcanic SO<sub>2</sub> product of S5P/TROPOMI based on detailed field observations from air, ground and the sea.**

*Dr. Santiago Arellano<sup>1</sup>, Dr. Nicolas Theys<sup>2</sup>, Dr. Bo Galle<sup>1</sup>, Dr. Michel Van Roozendael<sup>2</sup>*

<sup>1</sup>*Chalmers University of Technology, <sup>2</sup>Royal Belgian Institute for Space Aeronomy*

In order to characterize the uncertainty in measurements of volcanic SO<sub>2</sub> by S5P/TROPOMI it is important to constrain, in as much detail as possible, the environmental conditions affecting the measurement. These include e.g. the altitude of the plume, the distribution of concentration of SO<sub>2</sub> at sub-pixel resolution, or the amount of ash and aerosols in the plume.

We present the results of a detailed field experiment to validate measurements of volcanic SO<sub>2</sub> by S5P/TROPOMI at Manam volcano, Papua New Guinea. This target was identified as one of the top-10 sources of volcanic SO<sub>2</sub> by OMI observations during 2005-2015 (Carn et al., 2017). The volcano is located in a remote island and has an altitude of about 1800 m ASL. During 20-27 May 2019 we conducted measurements of the emission of SO<sub>2</sub> and other gases from Manam, during a period of elevated activity that culminated with an explosive eruption in June 2019. Our measurements include remote sensing with UV-DOAS instruments in three configurations: a) traverses on-board a drone (at 1020 m ASL); b) traverses on-board a boat around the island; and c) scanning measurements from ground. We also conducted in-situ concentration measurements of SO<sub>2</sub> and other gases using the drone and a electrochemical sensor unit.

Manam presented a challenging case for measurements due to low wind speeds, undefined wind direction, strong updraft, and changing cloud cover. In spite of these conditions, we were able to obtain very precise measurements of the column density distribution a few km downwind the crater and compare this to corresponding measurements by S5P/TROPOMI. We also constrained plume altitude and gas concentration and found that ash emissions were negligible.

In this contribution we present a comparison of our field observations with those of S5P/TROPOMI. This allows to identify and quantify sources of uncertainty due to complicated measurement scenarios. Based on this experience, we layout a framework for a systematic validation using existing ground-based instruments and dedicated field campaigns in around 40 volcanoes around the world.

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## Carbon Monoxide/Methane

### The Sentinel 5 Precursor CO and CH<sub>4</sub> operational data product: status and planning

Jochen Landgraf<sup>1</sup>, Alba Lorente<sup>1</sup>, Tobias Borsdorff<sup>1</sup>, Joost aan de Brugh<sup>1</sup>, Otto Hasekamp<sup>1</sup>, Maarten Sneep<sup>2</sup>, Bavo Langerock<sup>3</sup>, Mahesh Sha<sup>3</sup>

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The TROPOMI instrument of the Copernicus Sentinel 5 Precursor mission measures Earthshine reflectance spectra from the ultraviolet (UV) to the shortwave infrared (SWIR) spectral region. One of the primary objectives of the mission is to monitor the atmospheric trace gas carbon monoxide (CO) and methane (CH<sub>4</sub>) from the SWIR observations with unprecedented daily global coverage and a spatial high resolution of 5.5 × 7.5 km<sup>2</sup>. In this contribution, we summarize the current status of the CO and CH<sub>4</sub> operational data product, the routine validation and plans for future algorithm updates.

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### Sentinel-5P methane and carbon monoxide product validation using global TCCON and NDACC-IRWG data (TCCON4S5P and MPC results)

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The Sentinel-5 Precursor (S-5P) mission with the Tropospheric Monitoring Instrument (TROPOMI) has been operational since October 2017. It provides daily global coverage of methane (CH<sub>4</sub>) and carbon monoxide (CO), amongst other species, with a high spatial resolution. The S-5P CH<sub>4</sub> standard and bias-corrected products are currently available over land surfaces. The CO product is available over both land and water surfaces as an offline product as well as near-real-time product. Both the CH<sub>4</sub> and CO products have been validated using ground-based Total Carbon Column Observing Network (TCCON) data (standard and rapid delivery data) from the whole network as part of the ongoing TCCON4S5P project led by the Royal Belgian Institute for Space Aeronomy (BIRA-IASB) and using ground-based NDACC-IRWG (Network for the detection of Atmospheric Composition Change - Infrared Working Group) data from the whole network as part of the S-5P Mission Performance Centre. The validation results contributed significantly to the quantification of S-5P CH<sub>4</sub> and CO bias and precision, thereby leading to an official release of the products being recommended to European Space Agency (ESA).

In this presentation we will show the current validation results quantifying the biases with nearly two years of data. We will identify the cause of the biases based on the reference ground-based measurements from the TCCON and NDACC-IRWG sites. We will also discuss the remaining issues with the S-5P CH<sub>4</sub> and CO products.

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## **Validation of TROPOMI CH4 and CO using EM27/SUN and Aircore data in China**

*Prof. Zhaonan Cai<sup>1,2</sup>, Ms. Ke Che<sup>1,2</sup>, Prof. Yi Liu<sup>1,2</sup>, Prof. Dongxu Yang<sup>1,2</sup>, Ms. You Yi<sup>1,2</sup>*

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A compact travelling ground-based Fourier-transform spectrometer (EM27/SUN) and Aircore soundings were used to validate the CH4 and CO retrievals of TROPOMI onboard SSP in Beijing and Qinghai province (in northeastern part of Tibetan Plateau). The EM27/SUN interferogram was processed by PROFFAST algorithm and XCH4, XCO can be retrieved from these solar measurements. Aircore and corresponding soundings were launched in 2018 in Inner Mongolia and 2019 in Tibetan Plateau. Profiles of CO<sub>2</sub>, CH4, CO, N<sub>2</sub>O, O<sub>3</sub>, water vapor and aerosol particles are collected during these field campaigns. A temporal-spatial criteria of 30 minutes and 25 km was used to match EM27/SUN and TROPOMI measurements. For CO, the bias is -1.58±7.10% with correlation coefficient of 0.96 in Beijing, with coincident data from Jan to July 2019. In Qinghai, six coincident pairs were collected from July 15 to August 10, and there is a significant systematic bias of 39% with correlation coefficient of 0.78. For CH4, the bias is 8.5 ppb with a standard deviation of 11 ppb and the correlation coefficient is 0.85 in Beijing. There is no CH4 coincident pairs of EM27/SUN and TROPOMI that satisfy the criteria during the Qinghai field campaign, however, three EM27-GOSAT coincident pairs shows small negative biases. The aircore data were used to estimate the effect of profile in the column mixing ratio retrievals of CH4 and CO using EM27/SUN. The results indicate SZA-dependent biases of a few ppb for CH4 and CO.

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## **Comparisons of TROPOMI CH4 measurements with ACE-FTS**

*Mr. Tyler Wizenberg<sup>1</sup>, Prof. Kimberly Strong<sup>1</sup>, Prof. Kaley Walker<sup>1</sup>, Mr. Sebastien Roche<sup>1</sup>, Dr. Claus Zehner<sup>2</sup>, Dr. Ilse Aben<sup>3</sup>, Dr. Jochen Landgraf<sup>3</sup>*

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The Atmospheric Chemistry Experiment (ACE) Fourier transform spectrometer (FTS) is a high-spectral-resolution (0.02 cm<sup>-1</sup>) interferometer that was

launched aboard the Canadian SCISAT satellite in August 2003. Since 2004, it has been making solar occultation limb measurements from which trace-gas profiles are retrieved. It is currently one of the only satellite-borne instruments that is capable of retrieving atmospheric profiles of CH4 at high vertical resolution. In this work, we compare global TROPOMI CH4 data products with ACE-FTS to quantify how closely the TROPOMI measurements correlate with those from ACE-FTS. We convert ACE-FTS vertical volume mixing ratio profiles into column-averaged dry-air mole fractions to enable comparisons of the measurements from these two instruments. Measurements of CH4 made by a Bruker IFS 125HR Fourier transform infrared spectrometer located at the Polar Environment Atmospheric Research Laboratory (PEARL) at Eureka, Nunavut (80°N, 86°W) are also included in the comparisons for additional context.

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## **Sentinel-5 Precursor methane and carbon monoxide columns: Comparisons of scientific WFM-DOAS and operational retrievals**

*Dr Michael Buchwitz<sup>1</sup>, Dr Oliver Schneising<sup>1</sup>, Dr Maximilian Reuter<sup>1</sup>, Dr Heinrich Bovensmann<sup>1</sup>, Prof Dr John P. Burrows<sup>1</sup>, Ms Ann-Kathrin Krutsch<sup>1</sup>*

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Among the operational data products, retrieved from the measurements of the TROPOMI instrument on board the European Sentinel-5 Precursor (SSP) satellite, are methane (CH4) and carbon monoxide (CO) vertical columns. The methane data products is the column-averaged dry-air mole fraction, denoted XCH4, and that of CO is the CO vertical column in number of CO molecules (in moles) per unit area. At the University of Bremen, an independent retrieval algorithm called WFM-DOAS (or WFMD) has been developed and the first global data sets of XCH4 and XCO (column-averaged dry-air CO mole fraction) have been generated covering the period November 2017 to end of 2018.

The availability of a (scientific) data product generated independently facilitates research applications. In addition and in combination with the operational ESA/EU Copernicus product, it offers several interesting and important research options, such as the assessment of the robustness of critical higher-level product, such as derived surface fluxes (emissions and deposition/uptake). An important application for these products is to use them to detect spatial pattern of elevated atmospheric concentrations and to quantify the emissions from (corresponding) localized emission

sources using approaches such as mass balance methods. Each retrieval algorithm uses particular assumptions and approximations on which the resulting products and its characteristics always depend. This is not only with respect to the retrieved value of the main parameter (e.g., XCH<sub>4</sub>) but also with respect to its estimated uncertainty, its averaging kernel and its spatio-temporal coverage (due to different algorithm specific quality filtering approaches).

In this presentation, we introduce the WFMD algorithm and present comparisons of the generated WFMD data products with ground-based XCH<sub>4</sub> and XCO retrievals from the Total Carbon Column Observing Network (TCCON) and with the corresponding operational S5P data products. Details are given in the following publications (both Schneising et al 2019, which are in review): "Devastating Californian wildfires in November 2018 observed from space: the carbon monoxide perspective" (<https://doi.org/10.5194/acp-2019-5>) and "A scientific algorithm to simultaneously retrieve carbon monoxide and methane from TROPOMI onboard Sentinel-5 Precursor" (<https://doi.org/10.5194/amt-2019-243>).

The WFMD algorithm will be iteratively improved and used to generate improved data sets (e.g., extended time coverage). After assessment of their accuracy and after the generation of all relevant documentation (e.g., a user guide), the S5P WFMD XCH<sub>4</sub> product will be made available in the framework of the GHG-CCI+ project of ESA's Climate Change Initiative (CCI).

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### **Retrieving methane total column from TROPOMI measurements: algorithm improvements and validation results**

*Alba Lorente<sup>1</sup>, Tobias Borsdorff<sup>1</sup>, Joost aan de Brug<sup>1</sup>, Andre Butz<sup>2</sup>, Bavo Langerock<sup>3</sup>, Mahesh K. Sha<sup>3</sup>, Otto Hasekamp<sup>1</sup>, Jochen Landgraf<sup>1</sup>*

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The TROPOspheric Monitoring Instrument (TROPOMI) aboard of the Sentinel 5 Precursor (S5P) satellite measures the abundance of methane, the second most important anthropogenic greenhouse gas in the atmosphere. The operational CH<sub>4</sub> retrieval algorithm provides column averaged dry air volume mixing ratio of CH<sub>4</sub> from backscatter radiances measured by TROPOMI in the near-infrared (NIR, 675-775 nm) and shortwave-infrared (SWIR, 2305-2385 nm) spectral range while accounting for atmospheric scattering with the RemoTeC full-physics retrieval algorithm. In this

contribution we present the status of the TROPOMI CH<sub>4</sub> product with the focus on the latest developments of the retrieval algorithm that will be implemented in the next update of the operational processor. We implemented a new regularization scheme that led to a more stable inversion and a weaker dependence on the retrieved surface albedo. The remaining albedo dependence posterior to the retrieval is corrected using a more sophisticated method that derives the correction only from TROPOMI CH<sub>4</sub> data itself. These developments result in an improved data quality, as shown by a detailed validation of more than one year of TROPOMI CH<sub>4</sub> measurements with ground-based measurements by the TCCON network. The validation indicates a slight overestimation of the TROPOMI CH<sub>4</sub> corrected product with respect to TCCON observations, with a bias of 7.2 ppb and station-to-station variability of 3.9 ppb, the latter having decreased by almost a factor of 2 with respect to the current data release. The mean scatter of the bias is 13.2 ppb, which marginally varies between TCCON sites. Beyond the precision calculated by the retrieval algorithm, the validation results serve as a benchmark to characterize the uncertainty of the TROPOMI CH<sub>4</sub> for data assimilation and inversion studies. Further future updates include retrievals for observations over ocean in sun-glint geometry which we compare to results from a non-scattering retrieval and validate with ground-based measurements. The preliminary application of a de-striping algorithm is discussed to remove the row-dependent biases in the TROPOMI CH<sub>4</sub> product.

## Low-resolution FTIR spectrometers for the validation of S-5P CH<sub>4</sub> and CO products

*Dr. Mahesh Kumar Sha<sup>1</sup>, Martine De Mazière<sup>1</sup>, Justus Notholt<sup>2</sup>, Thomas Blumenstock<sup>3</sup>, HuiLin Chen<sup>4</sup>, Angelika Dehn<sup>5</sup>, David W. T. Griffith<sup>6</sup>, Frank Hase<sup>3</sup>, Pauli Heikkilä<sup>7</sup>, Christian Hermans<sup>1</sup>, Marko Huebner<sup>8</sup>, Nicholas Jones<sup>6</sup>, Rigel Kivi<sup>7</sup>, Bavo Langerock<sup>1</sup>, Christof Petri<sup>2</sup>, Qiansi Tu<sup>3</sup>, Damien Weidmann<sup>8</sup>*

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Nadir viewing satellite instruments provide global measurements of target species which rely on high-quality reference data for validation. The ground-based TCCON and the NDACC-IRWG networks have been the key facilities for the validation of satellites measuring greenhouse (CO<sub>2</sub> and CH<sub>4</sub>) and pollution (CO) gases. However, the number of stations available worldwide is limited and thus leaving large measurement gaps. Therefore a denser distribution of ground-based solar-absorption measurements covering different surface conditions (albedo), and a wide latitudinal and seasonal distribution are needed. For this reason, several groups are investigating alternative portable low-cost instruments, which can complement the existing networks and thus enhance the validation of satellite measurements.

The ongoing European Space Agency (ESA) funded campaign “Fiducial Reference Measurements for Ground-Based Infrared Greenhouse Gas Observations (FRM4GHG)” at the Sodankylä (Finland) TCCON site aims at the assessment of several low-cost portable spectrometers for the precise measurement of CO<sub>2</sub>, CH<sub>4</sub> and CO. These measurements have been performed simultaneously next to the TCCON instrument since 2017. In addition, regular AirCore launches were performed from that site providing in-situ reference profiles of the target gases; these are useful for the verification of the instrument calibration. The intercomparison results show that the low-resolution instruments tested could provide high quality data comparable to that of TCCON. The data collected during the campaign were used for the validation of CH<sub>4</sub> and CO measured by the Sentinel-5P satellite mission. The validation results will be presented and the added value of portable FTIR spectrometers will be discussed.

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## Physics based machine learning for Sentinel 5P SWIR retrieval validation

*Dr Edward Malina<sup>1</sup>, Dr Jennifer Adams<sup>2</sup>, Dr Ben Veihelmann<sup>1</sup>*

<sup>1</sup>ESA/ESTEC, <sup>2</sup>ESA/ESRIN

Methane is one of the key targets of the Sentinel 5P (S5P) TROPospheric Monitoring Instrument (TROPOMI), due to its significant impact on climate change. The operational S5P methane product is based on ‘optimal estimation methods’ using computationally expensive on-line radiative transfer forward simulations. Machine learning methods are computationally efficient in operational use, and require heavy computing power only whilst training. Machine learning methods can be employed to avoid on-line radiative transfer forward simulations and hence to speed up the methane retrieval from S5P. This provides an opportunity for using more advanced physics in this kind of retrievals and for providing a source of additional reference products for the validation of the operational S5P methane product.

This study is fundamentally based around ‘physics aware’ machine learning. In this case ‘physics-aware’ means the machine learning tool is emulating a well-known physical process, i.e. providing a statistical approximation of the transmission of electromagnetic radiation through the atmosphere, which can be modelled by Radiative Transfer Models (RTMs). Running complex forward RTMs are often the bottleneck in remote sensing, particularly in the provision of operational and/or near-real time products. Emulators of RTMs through machine learning are gaining much interest recently, due to the computational and timing gains they can achieve. Emulation of RTMs are being used increasingly within retrievals schemes for both multi- and hyper-spectral remote sensing, as well as for Look-Up-Table generation (e.g. for atmospheric correction) and sensitivity analyses.

In this work, we aim to validate the current S5P/TROPOMI SWIR trace gas products by developing SWIR trace gas products, based on a physics aware machine-learning algorithm, developed to accurately emulate S5P shortwave infrared (SWIR) spectra. The training dataset is comprised of a 50,000 state vectors of atmospheric parameters representative of any geolocation that S5P may encounter, and the resulting synthetic spectra, generated using the RemoTeC tool developed at SRON. The synthetic spectra provide a realistic approximation of the instrument response of S5P SWIR band, given a wide range of atmospheric

parameters, including scattering by aerosols and variations in surface albedo and solar zenith angle.

An emulator is then generated on the synthetic spectra training database, based on a Neural Network (NN) algorithm (using python's open-source 'scikit-learn'), in order to learn the physics of the LINTRAN RTM within the RemoTeC algorithm. Different NN architectures are tested to find the best performing NN, and resulting emulator. In our study, we find that the NN algorithm can effectively emulate TROPOMI SWIR spectra, explaining 99% of the variance, with low levels of Root Mean Squared Error (RMSE) when compared against the validation dataset for most cases. In addition to the development of the NN, effort was focused on uncertainty quantification for the algorithm given the necessity to provide uncertainty characterisation for S5P/TROPOMI SWIR products. Various methods exist since uncertainty quantification is becoming increasingly necessary. We will present preliminary results of our first approach to quantify uncertainty from the NN, focusing on a simple method based on calculating the Jacobian Covariance during the inference phase (i.e. application of emulator on the validation dataset).

This talk will detail the generation of the training and validation datasets, the selection of NN model architecture, and overall performances of the algorithm. We will cover how our results vary depending on what NN architecture is used, and how we assess the validity of the results output by the tool which is the current key drawback of NNs due to their black box nature. In this context, other methods of machine learning and/or uncertainty quantification will also be discussed (for example Gaussian Process Regression or Deep Bayesian Learning) to overcome the black-box nature of NNs. Finally, we will cover how physics aware machine learning can be incorporated into an optimal estimation retrieval architecture in order to generate Level-2 products.

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### **Qualitative Validation of TROPOMI L2 CO, NO<sub>2</sub>, and AI Products for use in Tracking the Impacts of Fire Emissions Plumes on Ambient Air Quality in the US**

*Dr. Amy Huff<sup>1</sup>, Dr. Shobha Kondragunta<sup>2</sup>*

<sup>1</sup>IMSG at NOAA/NESDIS/STAR, <sup>2</sup>NOAA/NESDIS/STAR

The suite of trace gas and aerosol products from the Tropospheric Ozone Monitoring Instrument (TROPOMI) on the Sentinel 5 Precursor (S5P) satellite is revolutionizing ambient air quality forecasting in the United States (US). TROPOMI provides – for the first time – critical information on the chemical composition of transported plumes with high spatial resolution. Key

TROPOMI level 2 (L2) near real-time products relevant for ambient air quality include measurements of carbon monoxide (CO), nitrogen dioxide (NO<sub>2</sub>), and the absorbing aerosol index (AI). A particular concern for air quality in the US is the growing impact of extreme wildfires. Fires directly emit primary fine particulate matter (PM2.5) in the form of smoke aerosols, and they also release large amounts of nitrogen oxides (NO<sub>x</sub>; sum of NO and NO<sub>2</sub>) and volatile organic compounds (VOCs), which are precursors for secondary formation of PM2.5 and ozone (O<sub>3</sub>). Smoke and emissions plumes from extreme fires can be transported long distances, degrading PM2.5 or O<sub>3</sub> air quality in locations far downwind. It can be difficult for operational air quality forecasters to predict whether a transported fire plume will be more O<sub>3</sub>-enhancing (optically thin, high in NO<sub>x</sub>) or primary PM2.5-enhancing (optically thick, high in smoke aerosols), since these effects are typically mutually exclusive. TROPOMI products will help distinguish between the two types of transported plumes: TROPOMI NO<sub>2</sub> should be high in O<sub>3</sub>-enhancing plumes, while TROPOMI AI should be high in PM2.5-enhancing plumes. TROPOMI CO is expected to be an overall tracer of both optically thick and thin fire emissions plumes. Examples will be presented from North American wildfire transport episodes in 2019, demonstrating qualitative validation of TROPOMI L2 products for tracking the impacts of transported fire emissions plumes on PM2.5 and O<sub>3</sub> air quality. Initial feedback on TROPOMI L2 products from operational end users in the U.S. will also be provided.

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## Nitrogen Dioxide

### The TROPOMI NO<sub>2</sub> product: validation, recent updates and development plans

*Dr. Henk Eskes<sup>1</sup>, Kai-Uwe Eichman<sup>2</sup>, Jos van Geffen<sup>1</sup>, Maarten Sneep<sup>1</sup>, Mark ter Linden<sup>1,3</sup>, Tijl Verhoelst<sup>4</sup>, Steven Compernolle<sup>4</sup>, Sander Niemeijer<sup>3</sup>, Pepijn Veefkind<sup>1</sup>*

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In our contribution we will review changes made to the NO<sub>2</sub> product in recent updates, the impact of the L1B upgrade, the major validation findings, major aspects influencing the quality of the product and development work for the upcoming updates.

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### Verification of TROPOMI S5p NO<sub>2</sub> columns with the scientific IUP Bremen product

*Dr. Andreas Richter<sup>4</sup>, Kezia Lange<sup>1</sup>, Prof. John P. Burrows<sup>1</sup>*

<sup>1</sup>University of Bremen

The excellent spatial resolution and good signal to noise of the TROPOMI instrument on S5p make it a very good instrument for tropospheric NO<sub>2</sub> retrievals. Local sources, individual pollution plumes and the effect of long-range transport of NO<sub>2</sub> can readily be seen in daily maps of the operational NRT and offline S5p NO<sub>2</sub> product.

While validation of the S5p NO<sub>2</sub> data set is best performed by comparison with ground-based and airborne data, it is also interesting to compare the operational data set with the scientific S5p NO<sub>2</sub> product retrieved at the University of Bremen. While the overall approach in NO<sub>2</sub> retrieval is similar between the two products, many of the detailed settings and assumptions applied are different, such as the spectral range used, the numerical method involved in determining the slant columns, the approach to stratospheric correction and the data bases applied as a priori in the air mass factor calculations.

By comparing the two products, an overall estimate of the uncertainty introduced by specific choices made in the retrieval can be provided, for example for the selection of spectral region used. The comparison highlights areas where the operational product is

strong, for example in the stratospheric correction, where improvements would be possible, for example in the spectral retrieval, and where updates in the data bases are needed, for example along coastlines and over pollution hotspots.

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### Comparison of TROPOMI/Sentinel 5 Precursor NO<sub>2</sub> observations with ground-based measurements in Helsinki

*Dr. Iolanda Lalongo<sup>1</sup>, Henrik Virta<sup>1</sup>, Henk Eskes<sup>2</sup>, Jari Hovila<sup>1</sup>, John Douros<sup>2</sup>*

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We present a comparison between satellite-based TROPOMI (TROPOspheric Monitoring Instrument) NO<sub>2</sub> products and ground-based observations in Helsinki (Finland). TROPOMI NO<sub>2</sub> total (summed) columns are compared with the measurements performed by the Pandora spectrometer during April–September 2018. We find a high correlation ( $r = 0.68$ ) between satellite- and ground-based data, but also that TROPOMI total columns underestimate ground-based observations for relatively large Pandora NO<sub>2</sub> total columns, corresponding to episodes of relatively elevated pollution. This is expected because of the relatively large size of the TROPOMI ground pixel (3.5 km x 7 km) and the a-priori used in the retrieval compared to the relatively small field-of-view of the Pandora instrument. Replacing the coarse a-priori NO<sub>2</sub> profiles with high-resolution profiles from the CAMS chemical transport model improves the agreement between TROPOMI and Pandora total columns for episodes of NO<sub>2</sub> enhancement.

We also analyse the consistency between satellite-based data and in situ NO<sub>2</sub> surface concentrations measured at the Helsinki-Kumpula air quality station (located a few metres from the Pandora spectrometer). We find similar day-to-day variability between TROPOMI, Pandora and in situ measurements, with NO<sub>2</sub> enhancements observed during the same days. Both satellite- and ground-based data show a similar weekly cycle, with lower NO<sub>2</sub> levels during the weekend compared to the weekdays as a result of reduced emissions from traffic and industrial activities (as expected in urban sites). The TROPOMI NO<sub>2</sub> maps reveal also spatial features, such as the main traffic ways and the airport area, as well as the effect of the prevailing south-west wind patterns.

This is one of the first works in which TROPOMI NO<sub>2</sub> retrievals are validated against ground-based observations and the results provide an early evaluation of their applicability for monitoring pollution levels in urban sites. Overall, TROPOMI retrievals are valuable to complement the ground-based air quality data (available with high temporal resolution) for describing the spatio-temporal variability of NO<sub>2</sub>, even in a relatively small city like Helsinki.

Reference: Ialongo, I., Virta, H., Eskes, H., Hovila, J., and Douros, J.: Comparison of TROPOMI/Sentinel 5 Precursor NO<sub>2</sub> observations with ground-based measurements in Helsinki, *Atmos. Meas. Tech. Discuss.*, <https://doi.org/10.5194/amt-2019-329>, in review, 2019.

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#### Evaluation of TROPOMI Tropospheric NO<sub>2</sub> VCDs over Xuzhou, China

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<sup>1</sup>China University Of Mining And Technology, <sup>2</sup>German Aerospace Center

The TROPOspheric Monitoring Instrument (TROPOMI) is a push broom UV-VIS-NIR-SWIR spectrometer carried on the Sentinel-5 Precursor (S5P) satellite which was launched on October 13th, 2017. Compared to onboard instruments such as GOME-2 and OMI, TROPOMI provides nitrogen dioxide (NO<sub>2</sub>) data product with higher spatial resolution, up to a ground pixel size of 3.5km × 7km at nadir. In this study, we evaluated the offline/reprocessing tropospheric NO<sub>2</sub> vertical column densities (VCDs) retrieved from TROPOMI between 2018-05-01 and 2019-07-31 (version 1.2 and 1.3) by using ground-based Multi AXis Differential Optical Absorption Spectroscopy (MAX-DOAS) in Xuzhou (a city in eastern China) and OMI NO<sub>2</sub> product produced by QA4ECV project. The comparison shows that the TROPOMI tropospheric NO<sub>2</sub> VCDs correlate well with the MAX-DOAS data with the Pearson correlation coefficient (*R*) of 0.87 after choosing the best quality assurance value (*qa\_value*=1). However, the underestimation of satellite NO<sub>2</sub> VCDs is up to 48% compared to MAX-DOAS data. The presence of cloud does affect the result of validation, especially when the cloud fraction is more than 60%. Besides that, we mapped the spatial distribution of TROPOMI and OMI NO<sub>2</sub> VCDs over high air-polluted regions such as Yangtze River Delta, Pearl River Delta, Jing-Jin-Ji Region, and Sichuan Basin during the period to compare their ability to distinguish contaminated areas. Meanwhile, the statistical data related to the urban economy such

as population, urban built-up area, and the number of vehicles were used to describe the spatial scale. The result shows that TROPOMI retrievals have proved to be able to describe air quality features and variability of the administrative division of a city even the NO<sub>2</sub> VCDs are high while OMI cannot show a clear difference.

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#### Using airborne- and ground-based high-resolution NO<sub>2</sub> columns to evaluate S5P TROPOMI Tropospheric NO<sub>2</sub> product

Dr. Laura Judd<sup>4,2</sup>, Dr. Jassim Al-Saadi<sup>1</sup>, Dr. Scott Janz<sup>3</sup>, Matthew Kowalewski<sup>3,4</sup>, James Szykman<sup>5</sup>, Dr. Lukas Valin<sup>5</sup>, Dr. R. Bradley Pierce<sup>6</sup>, Dr. Caroline Nowlan<sup>7</sup>, Dr. Gonzalo Gonzalez Abad<sup>7</sup>, Dr. Robert Swap<sup>3</sup>, Dr. Alexander Cede<sup>8</sup>

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High-resolution NO<sub>2</sub> columns retrieved from airborne spectrometer data (GeoTASO/GCAS) and ground-based Pandora columns are used to evaluate the Sentinel-5P (S5P) TROPOMI Tropospheric NO<sub>2</sub> Product near New York City and Long Island Sound. From June-October 2018, the GeoCape Airborne Simulator (GCAS) and GEOstationary Trace gas and Aerosol Sensor Optimization (GeoTASO) flew on NASA Langley Research Center aircraft during the daylight hours on 17 flight days under a variety of relatively clear-sky meteorological conditions. Flight times were optimized to maximize airborne measurements surrounding the S5P overpass time in the early afternoon which spans from 16:58-18:44 UTC over the flight domain. The 250 x 250 m aircraft NO<sub>2</sub> columns are extracted and mapped to coincident S5P TROPOMI pixels within an hour of the TROPOMI overpass. Preliminary results show that a few hundred TROPOMI pixels are over 75% mapped within that time period and are highly correlated to aircraft columns (*r*<sup>2</sup> > 0.90). However, in the spatial heterogeneous region of New York City and Long Island Sound, there is a low bias in the TROPOMI tropospheric vertical column product that is improved upon by recalculating tropospheric air mass factors using higher resolution a priori NO<sub>2</sub> profile shape factors. These results are also reflected by comparisons to a network of 10 Pandora spectrometers operating in the domain. Additional investigations are extended to other a priori factors like surface reflectivity and clouds. Results from this analysis are used to better understand S5P TROPOMI's ability to resolve NO<sub>2</sub> in urban/heterogeneous environments, and to continue refining techniques for the validation of future high-resolution space-based retrievals using airborne spectrometer observations to close the gap between

fixed ground-based validation platforms (e.g., Pandora) and satellite observations.

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## Nitrogen Dioxide

### Validation of TROPOMI S5P tropospheric NO<sub>2</sub> using ground-based MAX-DOAS and additional mobile DOAS campaign measurements

*Ms. Kezia Lange<sup>1</sup>, Mr. Andreas Richter<sup>1</sup>, Mr. Kai Krause<sup>1</sup>, Mr. Ilias Bougoudis<sup>4</sup>, Mr. John P. Burrows<sup>1</sup>, Mr. Stefan F. Schreier<sup>2</sup>, Mr. Sebastian Donner<sup>3</sup>, Mr. Steffen Dörner<sup>3</sup>, Ms. Bianca Lauster<sup>3</sup>, Ms. Katharina Uhlmannsiek<sup>3</sup>, Mr. Thomas Wagner<sup>3</sup>, Mr. Alexis Merlaud<sup>4</sup>, Mr. Frederick Tack<sup>4</sup>, Ms. Ermioni Dimitropoulou<sup>4</sup>, Mr. Michel Van Roozendael<sup>4</sup>*

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Sentinel-5P with the instrument TROPOMI provides, the possibility to investigate horizontal variations of NO<sub>2</sub> on small scales such as individual cities, thanks to its high spatial resolution of 3.5 km x 7 km, which was reduced furthermore to 3.5 km x 5.5 km recently. The identification of different emission sources is therefore much easier compared to data from earlier satellite instruments. Validation of this high resolution NO<sub>2</sub> data set can be performed by comparisons to ground-based stationary and mobile remote sensing measurements. Horizontal variations of NO<sub>2</sub> distributions are investigated with these different data sets.

First measurement campaigns have been carried out to get a more exhaustive overview of the horizontal NO<sub>2</sub> distribution for a better validation of TROPOMI data, in addition to the existing stationary ground-based stations.

Since August 2018 three MAX-DOAS instruments are distributed in the city of Vienna to get a better characterization of the horizontal variations of tropospheric NO<sub>2</sub> in Vienna. In view of these good local conditions additional mobile car and ship DOAS measurements were performed by BIRA, MPIC and IUP-

Bremen during the EGU 2019 in April. First results will be presented.

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### Sentinel-5p Tropospheric NO<sub>2</sub> Data Assessment using MAXDOAS and Direct-Sun Measurements

*Ms Gaia Pinardi<sup>1</sup>, Steven Compernolle<sup>1</sup>, Michel Van Roozendael<sup>1</sup>, François Hendrick<sup>1</sup>, Henk Eskes<sup>2</sup>, Alexander Cede<sup>3</sup>, Martin Tiefengraber<sup>3</sup>, Andreas Richter<sup>4</sup>, Ankie Piters<sup>2</sup>, Thomas Wagner<sup>5</sup>, Sebastian Donner<sup>5</sup>, Julia Remmers<sup>5</sup>, Alkis Bais<sup>6</sup>, Hitoshi Irie<sup>7</sup>, Yugo Kanaya<sup>8</sup>, Michel Grutter<sup>9</sup>, Claudia Rivera<sup>9</sup>, Sander Niemeijer<sup>10</sup>*

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Within the S5P Validation Team, the AO project NIDFORVAL (S5P Nitrogen Dioxide and FORmaldehyde VALidation using NDACC and complementary FTIR and UV-Vis DOAS ground-based remote sensing data) has been focusing on assessing the quality of nitrogen dioxide (NO<sub>2</sub>) and formaldehyde (HCHO) Sentinel-5p TROPOMI products throughout the mission. In this presentation, tropospheric NO<sub>2</sub> RPRO and OFFL products from version 1.1.0 to 1.3.2 are verified through comparison with ground-based UV-Visible multi-axis DOAS (MAXDOAS) and direct-sun PANDORA remote sensing instruments. Updates of HCHO and stratospheric NO<sub>2</sub> validation results are presented in companion abstracts (Vigouroux et al. and Verhoelst et al.).

Owing to the multiple pointing geometries, the DOAS technique is sensitive to total, tropospheric and stratospheric NO<sub>2</sub> content. Under favorable conditions, MAXDOAS measurements can also provide coarse information on the vertical distribution of NO<sub>2</sub> in the low troposphere. They are thus a highly relevant source of correlative data for validation of nadir sensors such as S5p, that strongly rely on a-priori knowledge of the NO<sub>2</sub> vertical distribution. So far, MAXDOAS data have been collected at about 15 stations by the NIDFORVAL consortium partners.

Direct-Sun PANDORA spectrometers are sensitive to the total NO<sub>2</sub> columns. Data coming from the Pandoria Global Network (PGN) have been used in a demonstration phase within the NIDFORVAL project. In addition to this activity, PGN data from about 20 stations are now automatically ingested in the MPC CalVal VDAF webserver (<http://mpc-vdaf>-

server.tropomi.eu/no2) for the routine validation of S5p total NO<sub>2</sub> columns.

Here we investigate the consistency between the tropospheric NO<sub>2</sub> validation results obtained using MAXDOAS datasets and similar comparisons based on the PGN datasets. In the latter, the PGN tropospheric columns are derived by subtracting the S5p stratospheric content from the measured total columns. A special focus will be put on stations where both MAXDOAS and PANDORA measurements are performed.

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### **Global Assessment of TROPOMI NO<sub>2</sub> Data Using Improved OMI NO<sub>2</sub> Standard Product**

*Dr. Lok Lamsal<sup>1</sup>, Dr. Sungyeon Choi<sup>2</sup>, Dr. Sergey Marchenko<sup>2</sup>, Dr. Nickolay Krotkov<sup>3</sup>, Dr. Henk Eskes<sup>4</sup>*

<sup>1</sup>USRA/NASA GSFC, <sup>2</sup>SSAI/NASA GSFC, <sup>3</sup>NASA GSFC, <sup>4</sup>KNMI

We present a global assessment of the TROPOMI operational NO<sub>2</sub> product using a new NASA OMI NO<sub>2</sub> standard product (OMNO2, v4.0). The v4.0 incorporates a few important changes, and enhances data quality on a global scale through improvements in air mass factors that are used to convert retrieved slant to vertical column densities. The algorithm is based on MODIS-based, high-resolution, geometry-dependent Lambertian surface equivalent reflectivity (GLER) operational product and a new consistently retrieved effective cloud fraction and O<sub>2</sub>-O<sub>2</sub> optical centroid cloud pressures. These improvements increase tropospheric NO<sub>2</sub> columns by up to 50% over highly polluted areas. We assess the TROPOMI NO<sub>2</sub> product in two ways: 1) by upscaling operational TROPOMI data to the OMI ground resolution, and 2) by applying OMI NO<sub>2</sub> algorithm to TROPOMI data. Our assessment suggests that the operational TROPOMI data are highly consistent with the new v4.0 OMI NO<sub>2</sub> product.

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### **Assessment of Sentinel-5p Stratospheric NO<sub>2</sub> Data using NDACC Zenith-Scattered-Light DOAS Measurements**

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*Puentedura<sup>6</sup>, Margarita Yela-Gonzalez<sup>6</sup>, Richard Querel<sup>7</sup>, Alexandre Gruzdev<sup>8</sup>*

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An accurate determination of the stratospheric column of NO<sub>2</sub> is not only needed for understanding stratospheric ozone distribution and trends, but it is also a prerequisite for (or a part of) a reliable determination of the tropospheric NO<sub>2</sub> column from nadir-viewing UV-visible spectrometers such as Sentinel-5p TROPOMI. Indeed, a nadir NO<sub>2</sub> measurement under cloud-free conditions is sensitive to the entire slant column and the quality of separation between stratospheric and tropospheric components determines the accuracy of the latter, especially in low-to-moderate pollution scenes.

In the operational production of the official S5p NO<sub>2</sub> data (L2\_NO2\_\_), this separation is performed using a data assimilation approach with a strong forcing over clean regions, i.e. where the total observed slant column contains almost solely stratospheric NO<sub>2</sub>. The Chemical Transport Model TM5 is run in either forecast mode (for the S5P NRTI product) or a few days later in analysis mode (for the S5P OFFL product).

We present here an assessment of the quality of the Sentinel-5p TROPOMI stratospheric NO<sub>2</sub> product (both NRTI and OFFL, processor versions 1.1.0 through 1.3.2), carried out within the context of ESA's Sentinel-5p Mission Performance Centre (MPC) and the S5PVT AO project NIDFORVal (Nitrogen Dioxide and FORmaldehyde Validation using NDACC and complementary FTIR and UV-Vis DOAS ground-based remote sensing data, #208607).

Because of their enhanced sensitivity to the stratospheric column and weaker sensitivity to tropospheric conditions, zenith-sky DOAS UV-visible measurements acquired during twilight are the reference measurements of choice. Over 30 zenith-scattered-light (ZSL) DOAS instruments perform network operation from pole to pole within the Network for the Detection of Atmospheric Composition Change (NDACC). Among them, 14 fully automated SAOZ instruments contribute data in near-real-time to the operational validation of S5p in the context of the MPC. About 10 other NDACC ZSL-DOAS instruments also contribute timely validation data through the NIDFORVal AO project. Most of those instruments have participated in the validation of stratospheric NO<sub>2</sub> from historical missions like GOME and SCIAMACHY, and current missions like OMI and GOME-2.

We describe the co-location scheme that deals with the large horizontal extent of the airmass to which a twilight zenith-sky measurement is sensitive, which differs significantly from the ground pixel size of TROPOMI data. We also describe the model-based adjustment that is performed to compensate for the photochemical changes of NO<sub>2</sub> between twilight and the S5p overpass time in the early afternoon.

We show that from the Arctic to the Antarctic S5p stratospheric NO<sub>2</sub> data follow closely the meridian structure and seasonal and shorter scale variability reported by NDACC ground-based observations. They correlate well with ground-based values under a variety of conditions ( $r > 0.9$  at most sites), both background and polluted, cloudy and clear, and under low sun or high sun, albeit with a slight overall negative bias of approximately 0.2 Pmolecules/cm<sup>2</sup>. The performance of S5p stratospheric NO<sub>2</sub> is briefly compared to that from other UV-visible satellites, such as the recently validated OMI QA4ECV and STREAM data sets.

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#### **Effect of Urban Boundary-layer turbulence on NO<sub>2</sub> tropospheric columns retrieved from Pandora-2S**

*Dr. Stefano Casadio<sup>1</sup>, Dr Anna Maria Iannarelli<sup>1</sup>, Dr. Marco Cacciani<sup>2</sup>, Dr. Annalisa di Bernardino<sup>2</sup>, Dr. Gabriele Mevi<sup>1</sup>*

<sup>1</sup>Serco Italia, <sup>2</sup>University Sapienza

The Boundary-layer Air Quality analysis Using Network of INstruments (BAQUNIN) super-site, active in the Rome area since 2017, is equipped with a large number of in situ and remote sensing instruments devoted to the retrieval of atmospheric parameters for satellite Cal/Val and urban atmosphere studies. The BAQUNIN suite comprises instruments participating in Pandoria Global Network (PGN), EUBREWNET, EUROSKYRAD and AERONET. In addition, we currently run a multi-wavelength lidar (polarisation included), a SODAR, a Pyranometer, a Sky-Camera, a MFRSR, a meteo station. In situ devices for the estimate of O<sub>3</sub>, NO<sub>2</sub>, NO, SO<sub>2</sub>, and CO surface concentrations are being tested and will be enter into operations by the end of 2019. Finally, a WRF model is run on daily basis to provide 36 hour forecasts at high temporal and spatial resolution.

In this work we present the results of a study focused on the assessment of the impact of urban surface-layer wind velocity on the amount of NO<sub>2</sub> Tropospheric Columns and Surface Concentrations (hereafter TC and SC) that can be retrieved from a Pandora-2S. For this activity we used the data produced by the SODAR and the Pandora #117 located at the Atmospheric Physics

laboratory (APL, Rome downtown). Both Pandora and SODAR are installed a few meter apart on the roof of the Physics Department of University Sapienza, at about 30 meters above the urban canopy layer.

The SODAR wind profiles have a time resolution of 10 minutes, while the Pandora is operated in a MaxDOAS mode, executing vertical scans for 0, 60, 120, 180, 240, 300 degrees (with respect to North) azimuth angles. The resulting time resolution for the retrieved TCs and SCs is about 7 minutes.

For this study, we averaged the SODAR horizontal wind intensity profiles in the first 100 meters altitude above the instrument, then we collocate SODAR and Pandora data in the temporal scale. The combined dataset has then been used to investigate the role of surface layer wind intensity on the upward NO<sub>2</sub> transport due to updrafts in relation with the turbulent development of the urban boundary layer.

Results clearly indicate that the inverse correlation between the wind intensity and the TC and SC is extremely high, with high TC and SC values in presence of low wind speeds. The TC and SC can be (quite accurately) described through a  $C = AxU^{-B}$  relationship, where "C" is the tropospheric or surface concentration, "A" and "B" constants, and "U" the wind speed in the surface layer.

The implications for the TROPOMI validation using Pandora-like spectrometers operating in urban areas is evident: the NO<sub>2</sub> concentration values retrieved from ground, and possibly from space, strongly depend on the urban canopy structure, the type of NO<sub>2</sub> sources (for the Rome case NO<sub>2</sub> is almost totally due to traffic) and on the urban boundary layer stability.

The BAQUNIN instrumental setup, the data analysis and the study results will be discussed in details.

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## Formaldehyde

### Current status and validation of the S5P

#### Formaldehyde L2 operational product

*Ms Isabelle De Smedt<sup>1</sup>, K.U Eichman<sup>2</sup>, S. Compernolle<sup>1</sup>, Z. Cheng<sup>3</sup>, N. Theys<sup>1</sup>, C. Ierot<sup>1</sup>, H. Yu<sup>1</sup>, J. Vlietinck<sup>1</sup>, F. Romahn<sup>3</sup>, P. Hedelt<sup>3</sup>, J.-C. Lambert<sup>1</sup>, D. Loyola<sup>3</sup>, M. Van Roozendael<sup>1</sup>*

<sup>1</sup>BIRA-IASB, <sup>2</sup>IUP-B, <sup>3</sup>IMF-DLR

The Sentinel-5 Precursor (S5P) was launched on the 13th of October 2017, with on board the TROPOMI instrument (TROPOMI). One year after the launch, the formaldehyde (HCHO) L2 product has been made operational.

The prototype of the tropospheric HCHO retrieval algorithm is developed at BIRA-IASB and implemented at the German Aerospace Center (DLR) in the S5P operational processor (De Smedt et al., 2018). The current version of the algorithm covers a period starting in May 2018 (RPRO v1.1.5) up to now (OFFL and NRT products v1.1.[5,6,7]). An update (v2) is currently under testing for the next release into the operational environment.

In this work, we present the quality of the HCHO product, its known issues and the updates foreseen in the next version. A summary of the validation results within MPC is presented. It includes satellite-satellite comparison with the OMI QA4ECV HCHO product and ground-based validation using MAX-DOAS instruments. Validation results are compared to the reported product uncertainties and statistics.

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#### Validation of TROPOMI HCHO observations over the US and over open ocean with SEAC4RS and ATom-4 aircraft mission data

*Dr. Jenny Stavrakou<sup>1</sup>, Dr. Jean-Francois Muller<sup>1</sup>, Dr. Maite Bauwens<sup>1</sup>, Dr. Isabelle De Smedt<sup>1</sup>, Dr. Michel Van Roozendael<sup>1</sup>*

<sup>1</sup>Royal Belgian Institute For Space Aeronomy

Satellite formaldehyde (HCHO) column data are widely used to constrain emissions of volatile organic compounds (VOCs), making the validation of these

datasets an urgent task. Our purpose is to evaluate HCHO columns from the TROPOMI instrument using highly accurate HCHO aircraft observations from two NASA aircraft missions : (1) the SEAC<sup>4</sup>RS (Studies of Emissions, Atmospheric Composition, Clouds and Climate Coupling by Regional Surveys) campaign over the southeast US in August–September 2013 and (2) the ATom-4 (Atmospheric Tomography Mission) deployed over the Atlantic and Pacific ocean in April-May 2018. We use the IMAGES global chemical-transport model at  $2^{\circ} \times 2.5^{\circ}$ , and the MAGRITTE regional model over the US at  $0.5^{\circ} \times 0.5^{\circ}$  as physical intercomparison platform for evaluating satellite columns against in situ measurements through model simulations. The southeast US is a well-known HCHO hot spot due to the enhanced HCHO production in summer from biogenic VOCs and especially isoprene. Over oceanic regions, the HCHO levels are generally very low as HCHO formation is mainly due to methane oxidation, although other NMVOCs might also contribute. Because the SEAC<sup>4</sup>RS data are not coincident with the TROPOMI observations, we use an adjoint-based technique to generate HCHO distributions matching the aircraft data, from which aircraft-based HCHO columns are derived. Those columns are used to assess the potential biases of OMI HCHO against SEAC<sup>4</sup>RS data over the U.S. Next, the TROPOMI HCHO columns are compared with OMI in summer 2018, in order to assess biases of TROPOMI data against both OMI and aircraft data, assuming that the interannual variability of HCHO columns is well represented by OMI data, as suggested by a recent modeling study.

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#### Validation of TROPOMI/S5P HCHO using UV-Vis DOAS and FTIR ground-based networks

*Dr. Corinne Vigouroux<sup>1</sup>, Bavo Langerock<sup>1</sup>, Gaia Pinardi<sup>1</sup>, FTIR and DOAS partners*

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As part of the S5P Validation Team, we will present the updated results of the NIDFORVal project (S5P Nitrogen Dioxide and Formaldehyde Validation using NDACC and complementary FTIR and UV-Vis DOAS ground-based remote sensing data), focusing on the formaldehyde (HCHO) S5P products.

In the NIDFORVal project, the HCHO retrieval settings have been optimized and harmonized at most of the FTIR (Fourier Transform Infrared) stations part of the Network for the Detection of Atmospheric Composition Change (NDACC), ensuring a consistent validation among the sites (Vigouroux et al., 2018). For the MAXDOAS (Multi-Axis Differential Optical Absorption Spectroscopy) stations, a best-effort basis harmonized

dataset is used so far, which will be improved and enlarged within another S5P Validation Team project (FRM4DOAS).

Data from sixteen FTIR sites and ten MAXDOAS stations were already used for the preliminary validation of the HCHO S5P columns (commissioning and pre-operational phase), providing a wide range of observation conditions including high, mid, and low latitudes, as well as remote, sub-urban, and urban polluted sites. The comparison results showed usually negative biases (TROPOMI being smaller) that were well within the accuracy requirements (40-80%). While the standard deviations were within the precision requirements for clean sites ( $1.2 \times 10^{16}$  molec/cm<sup>2</sup> for a single pixel), polluted sites showed larger deviations attributed to higher spatial/temporal variability.

This presentation will show extended results of our TROPOMI HCHO validation. First, the number of ground-based FTIR stations increases up to twenty-four, including world regions that were not covered before (Amazon basin, Japan, Oceania). Second, the TROPOMI time-series is getting longer: 17 months, from May 2018 to present day, for the validated products (RPRO + OFFL v.01.01.05 + OFFL v.01.01.06 + OFFL v.01.01.07). This enables the verification of the observed TROPOMI seasonal variability at many different sites around the globe. Furthermore, this extended validation allows us to discuss the provided random and systematic TROPOMI uncertainties.

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#### **Airborne Measurements of CH<sub>2</sub>O Obtained During the Long Island Sound Tropospheric Ozone Study (LISTOS): Comparisons with TROPOMI L2 product.**

*Dr. Scott Janz<sup>1</sup>, Mr. Matthew Kowalewski<sup>1</sup>, Dr. Laura Judd<sup>2</sup>*

<sup>1</sup>Nasa GSFC, <sup>2</sup>NASA LaRC

This overview will present details of vertical column formaldehyde measurements obtained from two airborne instruments deployed during the Long Island Sound Tropospheric Ozone Study (LISTOS) campaign in the summer of 2018. The GEO-CAPE Airborne Simulator (GCAS) and the Geostationary Trace Gas and Aerosol Sensor Optimization (GeoTASO) instruments are high spectral and spatial resolution push-broom spectrometers developed to measure trace gas column abundances in the atmosphere from aircraft for regional air quality studies and satellite validation/inter-comparisons. Details of the instrument will be presented including trace gas retrieval

sensitivities and uncertainties due to assumptions made in surface reflectivity and a priori chemical profiles in highly variable urban settings. Results under a variety of meteorological conditions will be described. Preliminary comparisons with the TROPOMI CH<sub>2</sub>O L2 product during the campaign time frame will be presented and show strong correlation with the aircraft product when the aircraft horizontal sub-samples are co-added to match the TROPOMI ground sample geometry.

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## **Uncertainty Characterisation**

#### **Towards Unified Error Reporting (TUNER)**

*Dr. Thomas von Clarmann<sup>1</sup>, Dr. Nathaniel J. Livesey<sup>2</sup>, Dr. Douglas A. Degenstein<sup>3</sup>*

<sup>1</sup>KIT/IMK, <sup>2</sup>NASA Jet Propulsion Laboratory/California Institute of Technology, <sup>3</sup>University of Saskatchewan  
The SPARC Activity "Towards Unified Error Reporting (TUNER)" aims at unification and harmonization of error analysis and reporting of satellite measurements of atmospheric state variables. Its goal is to make error estimates of existing satellite observations of atmospheric temperature and constituent profiles intercomparable. The main tasks within this project are (a) to develop a coherent terminology and formalism adequate to represent all existing retrieval schemes; (b) to assess the completeness of error budgets provided by the instrument teams of the relevant space missions; (c) to find ways to provide estimates of error components not considered so far and diagnostic data not provided so far, and (d) to develop recommendations how retrieval errors and other diagnostic data can be communicated to the user without generating unnecessary data traffic. In this talk the progress made will be reported, difficulties encountered will be discussed, and future plans will be presented.

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## **Reference Quality and Uncertainty in Atmospheric Measurements**

*Tom Gardiner<sup>1</sup>*

*National Physical Laboratory*

The GCOS Reference Upper Air Network (GRUAN) aims to provide reference quality measurements of key climate variables in the upper atmosphere through a global network of 20-30 sites. The measurements from the network provide data for long term climate trend determination and for the validation of more spatially extensive measurements such as satellites and the wider meteorological monitoring networks. A key element of the GRUAN measurement concept is that every data point is provided with information on its uncertainty. This talk will highlight some of the challenges in establishing traceability and uncertainty in atmospheric measurements and the tools being developed to address this. It will also discuss the importance of understanding the contribution of random and systematic components in the uncertainty budget, and how they evolve over different timescales.

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## **Uncertainty characterisation and harmonisation for Sentinel-5p products**

*Dr. Arno Keppens<sup>2</sup>, Dr. Steven Compernolle<sup>1</sup>, Dr. Tijl Verhoelst<sup>1</sup>, Dr. Daan Hubert<sup>1</sup>, Dr. Jean-Christopher Lambert<sup>1</sup>*

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The TROPOMI instrument on board of the Sentinel-5 Precursor mission acquires daily observations at unprecedented spatial resolution for an extensive list of atmospheric data products. These are retrieved by established product-specific algorithms that have been developed and are continuously being improved by several expert teams. Geophysical validation of the TROPOMI data products is also carried out by a large pool of experts contributing either to the Sentinel-5 Mission Performance Centre (MPC) or the S5PVT AO projects, or both. While the advantages of those unavoidably distributed development and validation are multiple, the downside is that uncertainty characterisation of both the data and of the data transformation process necessary to do data comparisons, is done following sometimes substantially different approaches. Therefore, in recent years, several international activities have addressed the harmonisation of atmospheric data uncertainties in various contexts, including the SPARC activity TUNER (Towards Unified Error Reporting), ESA CCI-ozone (Climate Change Initiative – Ozone ECV), and the EC projects QA4ECV (FP7) and GAIA-CLIM (H2020).

Applying the outcome of those previous activities to TROPOMI, the present work first provides an overview of the uncertainty characterisation approaches for the portfolio of TROPOMI atmospheric state variables – as described in their Algorithm Theoretical Baseline Documents (ATBDs) and Product Readme Files (PRFs) – and highlights where there is need and/or room for further harmonisation of the uncertainty reporting. Next, the most frequently used methods for this harmonisation of atmospheric state observations and their uncertainties are discussed in the context of TROPOMI level-2 data validation, where harmonisation of data representations in terms of physical quantities and vertical smoothing is needed. An overview of harmonisation or matching operations for atmospheric state observations is provided. The effect of these data manipulations on the information content of the original TROPOMI data and on the uncertainty budget of data comparisons is discussed.

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## Posters

### Characteristics of TROPOMI radiometric calibration analyzed with deep convective clouds over TWP region

*Ms. Yeeun Lee<sup>1</sup>, Prof. Myoung-Hwan Ahn<sup>1</sup>, Ms. Mina Kang<sup>1</sup>*

<sup>1</sup>*Ewha Womans University*

Since it is highly probable sensor characteristics might be changed over time after the launch of a satellite, comparing the sensor signals with other well-calibrated sensors can be a useful means of monitoring the accuracy of radiometric calibration during the operation. As one of sensors of GEO-constellation in the next decade, Geostationary Environmental Monitoring Spectrometer (GEMS) will provide UV-VIS hyperspectral data with similar observation conditions to the Band 3 and 4 of Tropospheric Monitoring Instrument (TROPOMI), a reciprocal candidate for the inter-calibration. GEMS is designed to observe the Tropical Western Pacific (TWP) region, and thus here we suggest deep convective clouds (DCCs) occurred in the region as a potential observation target for the inter-comparison. As a preliminary research, we compared the DCC reflectivity spectra observed by TROPOMI and Ozone Monitoring Instrument (OMI) and analyzed the signal trend in time-series to check whether the characteristics of radiometric calibration can be clearly seen in the DCC spectra of each sensor. To finely detect only DCCs having homogeneous radiative properties, we use IR window channel of Advance Himawari-8 Imager (AHI) based on the collocations with OMI and TROPOMI for the selection of the colder cloud tops. Results show that the spectral features of OMI and TROPOMI DCCs are almost well-matched with higher reflectivity (0.9 in average) except for the ozone absorption lines affected by the stratospheric ozone as well as the Fraunhofer lines. As the DCC reflectivity is calculated with the measured radiance and solar irradiance, degradation in the irradiance signal of OMI and TROPOMI slightly affects to the higher reflectivity especially in the shorter wavelengths. A certain amount of the degradation can be cancelled out in the reflectivity, though the spectral dependence caused by the degradation in the solar irradiance still remains especially in the TROPOMI signals. The systematic

difference between OMI and TROPOMI DCCs is shown nearly up to 10% depending on the different cloudiness and angle conditions and thus goniometry as well as the cloud properties of the DCCs are to be furtherly investigated. DCC selection also should be strictly performed to reduce the systematic difference among the DCC spectra, which will be presented as well in the study.

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### In-flight performance monitoring of TROPOMI Signal to Noise Ratio (SNR)

*Ms. Mijin Eo<sup>1</sup>, Prof Myoung-hwan Ahn<sup>1</sup>, Ms Mina Kang<sup>1</sup>*

<sup>1</sup>*Ewha Womans University*

Successful launch of the Tropospheric Monitoring Instrument (TROPOMI) onboard the Copernicus Sentinel-5 Precursor satellite provides global daily coverage of trace gases with high spatial resolution. The ratio of the corrected and useful signal to system noise signal of Level 1B (L1B) products is essential information for any product that use L1B data since accuracy on L1B depends on the achieved signal to noise ratio of the measurement. As signal to noise ratio (SNR) varies over time due to the instrumental effects such as instrument optical throughput, viewing condition and scene intensity, it is important to monitor the performance of SNR with sufficiently stable sources. Here, we estimate the SNR of UV-VIS band following in-flight SNR estimation method in general. The estimated SNRs using TROPOMI daily solar measurement within narrow range of solar elevation angle for May 2018 and binning over 11 wavelength steps are similar with given value from nominal measurement for a mid-latitude reference spectrum. It is challenging to estimate SNR directly from radiances because it is influenced by combination of viewing conditions and atmospheric conditions. Thus we estimate the SNR of Earth reflectance using the radiance from selected stable Earth scenes such as clouds, deserts and clear sky scene. The time series of SNR variability for each band of both irradiance and radiance from May 2018 to Oct 2019 will be presented to characterize the difference from each optical chain and monitor the short-term and long-term trend.

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## **Assessment of the quality of TROPOMI high-spatial-resolution NO<sub>2</sub> data products**

*Dr Xiaoyi Zhao<sup>1</sup>, Dr Debora Griffin<sup>1</sup>, Dr Vitali Fioletov<sup>1</sup>, Dr Chris McLinden<sup>1</sup>, Dr Alexander Cede<sup>2,3</sup>, Dr Martin Tiefengraber<sup>2,4</sup>, Dr Moritz Müller<sup>2,4</sup>, Dr Kristof Bognar<sup>5</sup>, Dr Kimberly Strong<sup>5</sup>, Dr Folkert Boersma<sup>6,7</sup>, Dr Henk Eskes<sup>6</sup>, Jonathan Davies<sup>1</sup>, Akira Ogyu<sup>1</sup>, Sum Chi Lee<sup>1</sup>*  
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Pandora NO<sub>2</sub> measurements made at three sites located in or north of the Greater Toronto Area (GTA) are used to evaluate the TROPOMI NO<sub>2</sub> data products, including standard Royal Netherlands Meteorological Institute (KNMI) tropospheric and stratospheric NO<sub>2</sub> data product and a TROPOMI research data product developed by Environment and Climate Change Canada (ECCC) using a high-resolution regional air quality forecast model (used in the air mass factor calculation). It is found that these current TROPOMI tropospheric NO<sub>2</sub> data products (standard and ECCC) met the TROPOMI design bias requirement. Using the statistical uncertainty estimation method, the estimated TROPOMI upper limit precision falls below the design requirement at a rural site, but above in the other two urban and suburban sites. The Pandora instruments are found to have sufficient precision to perform TROPOMI validation work. In addition to the traditional satellite validation method (i.e., pairing ground-based measurements with satellite measurements closest in time and space), we analyzed TROPOMI pixels located upwind and downwind from the Pandora site. This makes it possible to improve the statistics and better interpret the high-spatial-resolution measurements made by TROPOMI. By using this wind-based validation technique, the number of coincident measurements can be increased by about a factor of five. Using this larger number of coincident measurements, this work shows that both TROPOMI and Pandora instruments can reveal detailed spatial patterns (i.e., horizontal distributions) of local and transported NO<sub>2</sub> emissions, which can be used to evaluate regional air quality changes. The TROPOMI ECCC NO<sub>2</sub> research data product shows improved agreement with Pandora measurements compared to the TROPOMI standard tropospheric NO<sub>2</sub> data product, demonstrating benefits from the high-resolution regional air quality forecast model.

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## **Comparison of TROPOMI tropospheric NO<sub>2</sub> and HCHO VCDs to OMI and MAX-DOAS measurements in Munich**

*Dr. Ka Lok Chan<sup>1</sup>, Dr. Diego Loyola<sup>1</sup>, Dr. Matthias Wiegner<sup>2</sup>, Prof. Mark Wenig<sup>2</sup>*

<sup>1</sup>*German Aerospace Center, <sup>2</sup>Ludwig Maximilians Universität München (LMU)*

We present the comparison of TROPOMI measurements of NO<sub>2</sub> and HCHO vertical column densities (VCDs) to OMI and ground based MAX-DOAS measurements. The two dimensionally scanning MAX-DOAS measurements are performed in Munich, Germany. Tropospheric VCDs of NO<sub>2</sub> measured by TROPOMI agree well with the MAX-DOAS observations, with Pearson correlation coefficient (R) of 0.93. However, the absolute values measured by TROPOMI are ~30% lower. We have also compared TROPOMI HCHO VCDs to MAX-DOAS observations. The results show good agreement with R of 0.88 while TROPOMI observations are underestimated by ~25%. We have also evaluated the influences of a priori profile on satellite NO<sub>2</sub> and HCHO retrieval. MAX-DOAS observations of NO<sub>2</sub> and HCHO profile are used to recompute the air mass factors (AMFs) for satellite NO<sub>2</sub> and HCHO retrieval. The results show that the underestimation of NO<sub>2</sub> and HCHO VCDs is greatly improved when the MAX-DOAS profiles are used in the TROPOMI VCD retrieval. In addition, we have also analyzed the cloud dependency and spatial averaging effect. Furthermore, the spatial patterns of NO<sub>2</sub> and HCHO derived from OMI are compared to the TROPOMI observations.

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## **A new scientific data product of H<sub>2</sub>O/HDO columns from TROPOMI's short-wave infrared band and validation against TCCON**

*Dr. Andreas Schneider<sup>1</sup>, Dr. Tobias Borsdorff<sup>1</sup>, Dr. Joost aan de Brugh<sup>1</sup>, Dr. Alba Lorente Delgado<sup>1</sup>, Dr. Franziska Aemisegger<sup>2</sup>, Dr. Jochen Landgraf<sup>1</sup>*

<sup>1</sup>*Netherlands Institute For Space Research, <sup>2</sup>ETH Zürich*

A new scientific data set of vertical column abundances of the water vapour isotopologues H<sub>2</sub>O and HDO simultaneously retrieved from TROPOMI's short-wave infrared band is presented. Information about the isotopic composition of water vapour in the atmosphere is highly relevant, for example, for investigations on the hydrological cycle and how it changes with global warming. The retrieval is performed with the Shortwave Infrared CO Retrieval (SICOR) algorithm, which utilises a profile scaling approach. For validation, ground-based Fourier transform infrared (FTIR) measurements by the Total

Carbon Column Observing Network (TCCON) are employed. A comparison of TCCON  $\delta$ D with ground-based measurements by the project Multi-platform remote Sensing of Isotopologues for investigating the Cycle of Atmospheric water (MUSICA) for data prior to 2014 (where MUSICA data is available) reveals a bias in TCCON  $\delta$ D. As the TCCON HDO product is currently not calibrated or validated, an overall correction of recent TCCON HDO data is derived based on this finding. The agreement between the corrected TCCON measurements and collocated TROPOMI observations is good with an average bias of  $(-0.06 \pm 2) \cdot 10^{21}$  molec/cm<sup>2</sup> ( $(1.1 \pm 6.9)\%$ ) in H<sub>2</sub>O and  $(-0.8 \pm 6) \cdot 10^{17}$  molec/cm<sup>2</sup> ( $(-1.3 \pm 7.0)\%$ ) in HDO, which corresponds to a bias of  $(-15 \pm 19)\%$  in a posteriori  $\delta$ D. The value of this data set is demonstrated in the form of a short case study using single overpass data during a blocking anticyclone event in northeastern Europe.

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#### **Sentinel 5-Precursor cal/val activities near Bucharest, Romania**

*PhD Student Alexandru Dandocsi<sup>1</sup>, Dr. Anca Nemuc<sup>1</sup>, Dr. Dragos Ene<sup>1</sup>, Dr. Doina Nicolae<sup>1</sup>, Dr. Andreea Calcan<sup>2</sup>, Dr. Dirk Schuettemeyer<sup>3</sup>*

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The Sentinel 5-Precursor satellite with single carrying instrument onboard, TROPOMI, has been launched in October 2017 and since then it is providing daily coverage of methane (CH<sub>4</sub>), carbon monoxide (CO), nitrogen dioxide (NO<sub>2</sub>), and ozone (O<sub>3</sub>) among others. Preliminary validation of ground-based measurements of column-averaged abundances were provided by NDACC and TCCON, also COCCON network with their low resolution FTIR, for carbon monoxide and methane while for nitrogen dioxide and ozone column-averaged abundances are provided by Pandoria Global Network (PGN) and other MAX-DOAS instruments.

This presentation shows measurements from Magurele, Romania (44.35N, 26.03E) of a low spectral resolution FTIR, part of the COCCON initiative, regarding carbon monoxide and methane, and ozone and nitrogen dioxide retrievals from a Pandora-2S system, part of PGN. This location is of particular interest because it has urban influences from Bucharest and also rural influences being outside of the city in the southern part.

In the meantime, ESA is also interested in future space missions, geo-stationary missions like Sentinel 4 and other dedicated air pollution missions respectively. For that several projects are implemented by numerous scientific communities. RAMOS (Romanian Atmospheric Observation System) is a project aiming to develop a combination of ground-based and airborne remote sensing capabilities to retrieve several atmospheric species (greenhouse gases, air pollutants, aerosols). Romania's capabilities are exploited in order to develop a mobile platform (ground – based and airborne) which will be used to support the international efforts for calibration and validation of Earth Observation mission's products during both commissioning and operational phases. Further on RAMOS will be part of future ESA funded campaigns (QA4EO-Quality Assurance For Earth Observation) specially designed for cal/val activities. Main developments related to these projects will also be presented.

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#### **Synergistic Retrieval of Smoke, Dust, and Smog using SNPP VIIRS and S5P TROPOMI**

*Dr. Pubu Ciren<sup>1</sup>, Dr. Shobha Kondragunta<sup>2</sup>, Dr. Diego Loyola<sup>3</sup>*

<sup>1</sup>*IMSG Inc.&/NOAA/NESDIS/STAR,*

<sup>2</sup>*NOAA/NESDIS/STAR, <sup>3</sup>*German Aerospace Center (DLR)* NOAA Suomi National Polar Partnership (SNPP) Visible Infrared Imaging Radiometer Suite (VIIRS) aerosol detection product (ADP) identifies the presence of smoke and dust in the atmosphere. The ADP algorithm uses measurements at 412 nm, 440 nm, and 2.25  $\mu$ m to derive absorbing aerosol index (AAI) and Dust Smoke Discrimination Index (DSDI) to identify the presence of dust and smoke in the atmosphere. The ADP has been operational at NOAA since July 2017 and is shown to have 80% probability of correct detection (POCD) by comparing to Cloud Aerosol Lidar with Orthogonal Polarization (CALIOP) vertical feature mask (VFM). Aerosol Robotic Network (AERONET) Angstrom Exponent data are also used to classify the observations into smoke or dust based on certain criteria for coarse and fine mode particles.*

The NOAA proposed activity to European Space Agency (ESA) for Sentinel 5 Precursor Tropospheric Ozone Monitoring Instrument (S5P TROPOMI) calibration/validation activities includes exploring the possibility of a synergistic retrieval using measurements from VIIRS and TROPOMI to improve the accuracy of ADP and generate aerosol Detection product, that is capable of separate smoke and dust from observations of S5P TROPOMI. As a first step, NOAA JPSS VIIRS ADP algorithm is modified to be suitable for being applied to

the observations from S5P TROPOMI. Secondly, the required inputs are generated by using the synergy between SNPP VIIRS and S5P TROPOMI. Finally, The modified algorithm is applied to various cases, including smoke plumes from forest fires and dust outbreaks, for both local and transported events. Preliminary results indicate that TROPOMI ADP is able to identify smoke and dust both over land and ocean and matches with VIIRS ADP very well.

In this presentation, we will report the modified ADP algorithm by using synergy between SNPP VIIRS and S5P TROPOMI observations, comparisons of ADP from VIIRS with ADP from TROPOMI and validation against CALIOP VFM product.

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### **Improving the TROPOMI CO data product: update of the spectroscopic database and destriping of single orbits**

*Dr. Tobias Borsdorff<sup>1</sup>, Dr. Joost aan de Brugh<sup>1</sup>, Dr. Manfred Birk<sup>2</sup>, Dr. Georg Wagner<sup>2</sup>, Dr. Andreas Schneider<sup>1</sup>, Dr Alba Lorente<sup>1</sup>, Dr. Jochen Landgraf<sup>1</sup>*

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In this contribution we report on the planned updates to further improve the TROPOMI CO data set. The database of molecular absorption lines used in the TROPOMI CO retrieval will be changed to HITRAN2016 with the next processor update. By that the bias between TROPOMI CO and TCCON will be reduced from 6.2 ppb to less than 1 ppb and its station-to-station variability from 2.6 ppb to 1.8 ppb. Moreover, the update will improve the latitudinal bias between TROPOMI CO and the ECMWF CAMS-IFS model. To support this decision, we analyzed the effect of three further data sets for molecular absorption lines on the TROPOMI CO retrieval, HITRAN 2008, HITRAN2012, and the most recent line list of ESA's Scientific Exploitation of Operational Missions (SEOM) Improved Atmospheric Spectroscopy Databases (IAS) project and we discuss the impact of the different data sets on the CO data quality. Another planned update for the TROPOMI CO data product is a posteriori correction addressing the striping of single orbits in flight direction that can be easily applied by users of the level 2 data. We present two methods for the de-striping of the TROPOMI CO data one based on median filtering and the more advanced deploying a Fourier transform filtering of the data. The performance of the methods is discussed and quantified how much the dataset is changed by it. Finally, we will show examples of the application of the data set.

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### **Evaluation of the TROPOMI weekly cycles of NO<sub>2</sub> measurements over metropolitan areas using the long record of OMI observations and modeling**

*Dr Maite Bauwens<sup>1</sup>, Dr Jenny Stavrakou<sup>1</sup>, Dr Jean-François Müller<sup>1</sup>, Dr Folkert Boersma<sup>2</sup>, Dr Jos van Geffen<sup>2</sup>*

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Anthropogenic activities being by far the largest source of NO<sub>x</sub> into the atmosphere, reduced activity on rest days induces a weekly cycle in NO<sub>2</sub> abundances, with lower values observed on those days. Here we present a comprehensive analysis of the NO<sub>2</sub> weekly cycle over metropolitan areas on the global scale based on one full year of NO<sub>2</sub> observations (May 2018-April 2019) from the recently launched high-resolution TROPOMI sounder. Whereas most of the 300 cities included in this analysis shows a minimum (required to be at least 5% below the weekly mean) on Sunday (136), Friday (42), and Saturday (30) are also common. Among the remainder, 76 cities show a minimum on another weekday, and 16 cities do not show a clear minimum. Since the TROPOMI dataset covers only one year, meteorology-induced natural NO<sub>2</sub> variability has a strong impact on the mean weekly cycle, which explains the existence of deviations to the expected weekly cycle at a large number of cities, e.g. in Eastern Europe, Russia and even at several U.S. cities.

The TROPOMI-based weekly NO<sub>2</sub> cycle is compared to the weekly cycle derived based on OMI NO<sub>2</sub> column observations for the same year (2018) and further validated against the 2005-2017 OMI dataset. Comparisons with previous studies based on coarse-resolution spaceborne data and in situ measurements are discussed. The long record of OMI observations reveals trends in the weekly cycle resulting from changes in NO<sub>x</sub> emissions, either due to anti-pollution measures or to fast urbanization and industrialization. Indeed, clear evidence is found for a weakening of the NO<sub>2</sub> weekly cycle over European and U.S. cities, where the negative anthropogenic emission trends tend to lengthen the NO<sub>2</sub> lifetime, whereas the opposite is recorded in regions undergoing strong emission growth. Those effects are well described using multiyear model simulations.

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## **Sentinel5p NO<sub>2</sub> validation with the EMEP regional air quality model in the VALS-5p project**

*Dr. Michael Gauss<sup>1</sup>, Mr. Jan Griesfeller<sup>1</sup>, Dr. Svetlana Tsyro<sup>1</sup>*

<sup>1</sup>*Met Norway*

The presented poster will show validation of the tropospheric NO<sub>2</sub> column product of Sentinel-5p conducted for the VALS-5p project using data from the well established regional air quality model EMEP.

The goal of the project is to validate Sentinel-5p data against EMEP model data, as well as other satellite and ground-based measurements. Later on, the project will explore possibilities to assimilate Sentinel-5p data in the daily air quality forecasts for Europe and for Norway in particular, which the Norwegian Meteorological Institute is generating operationally with the EMEP model. Until now level-2 data of NO<sub>2</sub> columns from Sentinel-5p for the period March 2018 to present have been analysed.

NO<sub>2</sub> is mainly derived from road transport, energy production and distribution, energy use in the industry, services and households. Given its relatively short lifetime, most of the NO<sub>2</sub> resides in the lower troposphere and reflects the spatial distribution of emission sources fairly well. This also means that NO<sub>2</sub> columns correlate well with emission sources.

The EMEP model has been used for decades under the UN Convention on Long-range transboundary Air pollution (LRTAP) for several years in the Copernicus Atmosphere Monitoring Service (CAMS). It is evaluated regularly against measurements and the results are publicly available (e.g. EMEP reports, CAMS regional air quality website). According to the EMEP Status report 1/2019, the correlation of modeled NO<sub>2</sub> against measurements in the regional background was 0.84 and the bias -14%, which can be considered as a very good performance given the uncertainties in emission data. For the daily forecasts, and when urban background stations are taken into account the bias is smaller but the correlation is lower.

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## **Two years of worldwide inter-comparison of S5P/TROPOMI and SYNOP cloud fraction observations**

*Mr Chrysovalantis Sarakis<sup>1</sup>, Dr. MariLiza Koukouli<sup>1</sup>, Prof. Dimitrios Balis<sup>1</sup>, Dr. Diego G. Loyola<sup>2</sup>, Dr. Ronny Lutz<sup>2</sup>, Dr. Fabian Romahn<sup>2</sup>*

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In this study we examine the potential of cloud fraction (CF) observations reported as SYNOP from ground stations to validate satellite cloud observations from S5P/TROPOMI. Space borne retrieved cloud parameters help us understand the important effect clouds have on solar and terrestrial radiative scattering. Furthermore, the quality of the satellite cloud detection algorithms influence the estimation of space borne retrieved parameters, such as column densities and concentration profiles of atmospheric trace gas species. CF observations, reported in routine surface synoptic (SYNOP) bulletins, were used to validate the S5P/TROPOMI effective radiometric cloud fraction. The specific passive sensor is capable of cloud detection, using the Optical Cloud Recognition Algorithm (OCRA) / Retrieval Of Cloud Information through Neural Networks (ROCINN) algorithms, where Clouds are treated As Layers (CAL) and as Reflecting Boundaries (CRB). The retrieved CF has a spatial resolution of 7.2 x 3.5 km<sup>2</sup> and recently of 5.6 x 3.5 km<sup>2</sup>. The data quality value was set over 50 % for each S5P observation and a minimum 50% of data availability was requested for each SYNOP site. For the inter-comparison of each satellite pass the minimum distance between SYNOP site and TROPOMI was chosen (typically well-within the TROPOMI pixel) and within a 10 minute temporal difference from the collocating SYNOP observation. The TROPOMI Cloud product, between November 2017 and October 2019 was processed offline (OFFL). CF retrieved values were averaged both in time and space over the tropics, the middle-latitudes and the Polar regions. Results so far show that SYNOP reports are indeed a potent way of validating the S5P CF observations. In addition, it was found that linear correlation coefficients range between 0.54 and 0.80 and that there is an under-estimation of the S5P data by the corresponding SYNOP observations in high CF values as expected over the tropics, but further analysis has to be made.

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## **Carbon Monoxide Total Columns from Sentinel-5P Short-Wave Infrared Nadir Measurements**

*Mr Philipp Hochstaettler<sup>1</sup>, Dr. Franz Schreier<sup>1</sup>*

<sup>1</sup>*German Aerospace Centre (DLR)*

We present an assessment of carbon monoxide (CO) total column retrievals from TROPOMI (TROPOspheric Monitoring Instrument) Short-Wave Infrared (SWIR) observations aboard Sentinel-5P (S5P). The Level1-2 processing is accomplished by using the Beer Infrared Retrieval Algorithm (BIRRA) which performs a least squares fit of Earth's radiance (essentially transmission) to retrieve the molecular column densities (essentially

density scaling factors) along with some auxiliary parameters (reflectivity etc.) [Gimeno Garcia et al., AMT [011]. It has been developed at DLR since about 2005 and it's CO and CH<sub>4</sub> columns were thoroughly examined in several intercomparisons in the framework of DLR's SCIAMACHY activities [e.g. Hochstafl et al., Remote Sens. 2018]. The quality of our CO product is assessed through a comparison to data products from NDACC (Network for the Detection of Atmospheric Composition Change) and TCCON (Total Carbon Column Observing Network). Finally, we provide an updated description of BIRRA's current state (including its forward model GARLIC (Generic Atmospheric Radiation Line-by-line Infrared Code, Schreier et al. 2014)) and a brief overview of the updates in the BIRRA/TROPOMI processor framework.

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#### **Validation of Tropomi/Sentinel-5 Precursor Satellite Data Using Time Series of Ground-Based FTIR Sites at Different Latitudes**

*M.Sc. Amelie Ninja Röhling<sup>1</sup>, Dr. Thomas Blumenstock<sup>1</sup>, Dr. Frank Hase<sup>1</sup>, M.Sc. Ugur Cayoglu<sup>1</sup>, Dr. Omaíra E. Garcia<sup>3</sup>, Dr. Tobias Kerzenmacher<sup>1</sup>, Prof. Dr. Uwe Raffalski<sup>2</sup>, Dr. Eliezer Sepúlveda<sup>3</sup>*

<sup>1</sup>Karlsruhe Institute of Technology, <sup>2</sup>Swedish Institute of Space Physics, <sup>3</sup>State Meteorological Agency  
ESA's Sentinel-5 precursor satellite (S-5P) was launched in October 2017. It is an atmospheric composition satellite of the Copernicus programme, which carries the Tropospheric Monitoring Instrument (TROPOMI). The sensor measures, among other compounds, the trace gases carbon monoxide (CO), methane (CH<sub>4</sub>) and formaldehyde (HCHO) with high spatial resolution, providing important information on trace gas fields from the global down to the regional scale.

Ground based remote sensing observations are an important tool for the quality assurance of the datasets resulting from satellite missions. As part of the Network for the Detection of Atmospheric Composition Change (NDACC), we operate several ground-based infrared solar-absorption Fourier transform (FTIR) spectrometers for measuring the atmospheric concentrations of greenhouse gases, of stratospheric trace gases important for ozone chemistry, and several reactive tropospheric gases. The FTIR sites, used in this study, are located in Kiruna, Sweden (67.8°N, 20.4°E, 420m a.s.l.), in Karlsruhe, Germany (49.1°N, 8.44°E, 110m a.s.l.) and at the Izaña Observatory on Tenerife, Spain (28.3°N, 16.5°W, 2370m a.s.l.).

We will present a comparison between space-based TROPOMI and ground-based FTIR measurements. We will apply datasets of atmospheric column amounts of CO, CH<sub>4</sub> and HCHO collected at the aforementioned sites. These data have been generated by following the analysis procedures recommended by the NDACC. For methane and carbon monoxide, the ground-based measurements also provide limited information on the vertical distribution of the gases (two to three degrees of freedom). In addition, in-situ measurements of CO and CH<sub>4</sub> collected within the GAW (Global Atmospheric Watch) programme at the Izaña mountain observatory will be taken into account.

We will discuss the characteristics of the recorded ground-based time series and investigate the ability of S-5P of reproducing these features on different time scales. Moreover, we will make use of the wide swath width and high spatial resolution achieved by S-5P for discussing detected anomalies also in a spatial context.

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#### **Activities for the validation of TROPOMI Level 2 products by using GEMS algorithm and Ground-based network over East Asia**

*Sujung Go<sup>1</sup>, Professor Jhoon Kim<sup>1</sup>, Professor Myoung-Hwan Ahn<sup>2</sup>, Professor Chang-Keun Song<sup>3</sup>, Professor Jae Hwan Kim<sup>4</sup>, Professor Hanlim Lee<sup>5</sup>, Professor Rokjin Park<sup>6</sup>, Professor Sang-Woo Kim<sup>6</sup>, Professor Sang Seo Park<sup>3</sup>, Researcher Yukeun Ki<sup>1</sup>, Graduate Student Hana Lee<sup>1</sup>, Graduate Student Heesung Chong<sup>1</sup>, Graduate Student Mina Kang<sup>2</sup>*

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*Successful launch of the Tropospheric Monitoring Instrument (TROPOMI) onboard the Copernicus Sentinel-5 Precursor satellite to support the services and science related to air quality, climate and stratospheric ozone opens up a new possibility to provide the daily global concentrations of trace gases and aerosols with high spatio-temporal resolution. In this study, we tried to cross-validate the TROPOMI Level 2 products by utilizing algorithms prepared for the GEMS program and the data obtained from ground-based network over East Asia.*

For example, TROPOMI Level 2 operational products and GEMS Level 2 products simulated with Level 1B data of Sentinel-5p are compared for total ozone (total O<sub>3</sub>), nitrogen dioxide (NO<sub>2</sub>), sulfur dioxide (SO<sub>2</sub>), formaldehyde (HCHO), UV aerosol index, qualitatively over GEMS field of view (FOV). Overall, TROPOMI Level 2 operational algorithms and GEMS Level 2 algorithms captured the significant event very well and showed similar spatial distribution. However, the absolute values between two products showed slight differences possibly due to the algorithm differences including cross-section, surface albedo and spectral calibration. For total O<sub>3</sub> and NO<sub>2</sub>, TROPOMI operational products are validated with Pandora measurement data in Korea. For total O<sub>3</sub>, the correlation coefficient between TROPOMI operational products and Pandora measurement data are over 0.9 with about 6% bias. For NO<sub>2</sub>, there were significant correlation between TROPOMI operational products and Pandora measurement data with slight underestimation possibly due to local inhomogeneity of NO<sub>2</sub> emissions. Also, on March 4th, 2019, 12 products of GEMS Level 2 algorithms are simulated with Level 1B data of Sentinel-5p including products of O<sub>3</sub> profile, aerosol optical depth (AOD), single scattering albedo (SSA), UV Index. On March 4th, 2019, GOCI RGB and AOD showed high aerosol concentration in Korea with transportation from Eastern China. GEMS aerosol products retrieved with additional retrieval results of trace-gases in terms of spatial distribution will provide interesting case study over East Asia. This proves that TROPOMI Level 1B products shows reasonable performances for the Level 2 retrieval. Moreover, spatial distribution of carbon monoxide (CO) and NO<sub>2</sub> are analyzed in Korea using TROPOMI operational products. One-year periods of TROPOMI operational products are oversampled in 0.01° × 0.01° spatial resolution using tessellation approach. The results showed the common source between CO and NO<sub>2</sub> of South Korea.

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#### **Assessment of S-5p Tropospheric NO<sub>2</sub> Mapping and Impact of Spatial Smearing over Highly Polluted Regions Based on Coincident Airborne Apex Data**

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Sentinel-5 Precursor (S-5P), launched in October 2017, is the first mission of the Copernicus Programme dedicated to the monitoring of air quality, climate and ozone. Its characteristics, such as the fine spatial resolution, introduce many new opportunities and challenges, requiring to carefully assess the quality and validity of the generated data products by comparison with independent reference observations.

In the presented study, the S-5P/TROPOMI tropospheric nitrogen dioxide (NO<sub>2</sub>) product (3.5 × 7 km<sup>2</sup> at nadir observations) has been validated over strongly polluted urban regions based on comparison with coincident high-resolution airborne remote sensing observations (~100 m). Airborne imagers are able to map the horizontal distribution of tropospheric NO<sub>2</sub>, as well as its strong spatio-temporal variability, at high resolution and with high accuracy. Additionally, such data sets allow to study the TROPOMI subpixel variability and impact of signal smoothing due to its finite satellite pixel size, typically coarser than fine-scale gradients in the urban NO<sub>2</sub> field.

In the framework of the S5PVAL-BE campaign, the Airborne Prism EXperiment (APEX) imaging spectrometer has been deployed during four mapping flights (26–29 June 2019) over the two largest urban regions in Belgium, i.e. Brussels and Antwerp, in order to map the horizontal distribution of tropospheric NO<sub>2</sub>. Mapping flights and ancillary ground-based measurements (car-mobile DOAS, MAX-DOAS, CIMEL, ceilometer, etc.) were conducted in coincidence with the overpass of TROPOMI (typically between noon and 2 PM UTC). The TROPOMI and APEX NO<sub>2</sub> vertical column density (VCD) retrieval schemes are similar in concept and based on 1) Differential Optical Absorption Spectroscopy (DOAS) fitting of the pre-processed spectra in the visible wavelength region, 2) the calculation of appropriate air mass factors (AMFs) by a radiative transfer model in order to account for enhancements in the optical path length due to the surface albedo, aerosol and NO<sub>2</sub> profile shapes and viewing and sun geometry. Finally, retrieved NO<sub>2</sub> VCDs were georeferenced, gridded and intercompared. In Antwerp, main NO<sub>x</sub> sources are related to (petro)chemical industry in the harbour, while traffic emissions are dominant in Brussels. The NO<sub>2</sub> VCDs observed by APEX range between 3 and 35 × 10<sup>15</sup> and 1 and 20 × 10<sup>15</sup> molec cm<sup>-2</sup> in Antwerp and in Brussels, respectively. Per flight, 15 to 20 TROPOMI pixels were fully covered by approximately 5000 APEX measurements for each TROPOMI pixel. Averaging the APEX VCDs within a TROPOMI pixel reduces its uncertainty to 3.1 × 10<sup>13</sup>, a reduction by a factor of 22 when compared to the TROPOMI random uncertainty.

Preliminary results of the comparison and assessment of the TROPOMI tropospheric NO<sub>2</sub> product will be presented.

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### **Validation of Aerosol Layer Height retrieved from the TROPOMI / Sentinel-5 Precursor instrument using EARLINET lidar data**

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In this study we investigate the ability of the TROPOMI instrument on the Sentinel-5 Precursor satellite to deliver accurate geometrical features of lofted aerosol layers over the Europe. For this purpose, we use ground-based lidar measurements from European Aerosol Research Lidar Network (EARLINET) stations for validating the Aerosol Layer Height (ALH) product. The TROPOMI Aerosol Layer Height (ALH) is a new operational product and focuses on the retrieval of vertically localized aerosol layers in the free troposphere (desert dust, biomass burning aerosol and volcanic ash plumes) for cloud-free cases, which is derived from measurements of the oxygen A-band in the near infrared region between 758 nm and 770 nm. Knowledge of the ALH is essential for understanding the impact of aerosols on the climate system. Lidar instruments can provide aerosol profile information such as the backscatter and extinction coefficients at different wavelengths which are representative of the aerosol load, with a vertical resolution of a few meters. Currently, lidar networks, like the EARLINET monitor aerosol vertical distributions in the atmosphere. EARLINET includes 30 lidar stations and was established in 2000 as a research project with the goal of creating a quantitative, comprehensive, and statistically significant database for the horizontal, vertical, and temporal distribution of aerosols on a continental scale. The time period from March 2018 to September 2019 is selected for the comparison between satellite ALH Level-2 product and ground-based lidar backscatter profiles at 355, 532 and 1064nm. Spatiotemporal collocation criteria were set at a maximum of 150km and 6h. Collocated pixels, with significant aerosol load, were selected for cloud-free conditions and high values of UV Aerosol Index. The Mediterranean basin is a region affected strongly by Saharan dust transport and high levels of UV aerosol index indicating the presence

of dust aerosols layers. Data from EARLINET stations over Spain, Italy and Greece with good collocations with TROPOMI are used in this presentation for case studies to evaluate S5P/TROPOMI ALH for specific aerosol episodes.

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### **Gradients of greenhouse gases fields on regional scales observed with Sentinel-5P and COCCON spectrometers**

*Dr. Qiansi Tu<sup>1</sup>, Dr. Frank Hase<sup>1</sup>, Dr. Thomas Blumenstock<sup>1</sup>, Dr. Tobias Borsdorff<sup>2</sup>, Dr. Paolo Castracane<sup>3</sup>, Dr. Angelika Dehn<sup>3</sup>, Dr. Alba Lorente Delgado<sup>2</sup>, Dr. Pauli Heikkinen<sup>4</sup>, Dr. Rigel Kivi<sup>4</sup>, Dr. Jochen Landgraf<sup>2</sup>, Dr. Uwe Raffalski<sup>5</sup>, Dr. Mahesh Kumar Sha<sup>6</sup>*

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The Sentinel-5 Precursor (S5P) is the first mission of the Copernicus Programme, aiming at monitoring of air pollution, methane and the ozone layer with high spatio-temporal resolution (Veefkind et al., 2012). The mission fills in the gap between Envisat and Sentinel-5. The S5P satellite launched on 13 October 2017 and operates in a low Earth polar orbit, with an operational lifespan of seven years. Its single payload, the TROPOspheric Monitoring Instrument (TROPOMI) is a nadir-viewing grating spectrometer that covers wavelength bands from ultraviolet to shortwave infrared (SWIR). The SWIR module on TROPOMI allows the quantification of methane and carbon monoxide concentration in the Earth's atmosphere.

Column-averaged trace gas abundances as provided by the ground-based Fourier transform infrared (FTIR) networks Total Carbon Column Observing Network (TCCON) and Network for the detection of Atmospheric Composition Change – Infrared Working Group (NDACC-IRWG) are an important reference for the validation of space borne sensors. However, limited global coverage and station density of these networks leaves large gaps, especially at high latitude, in the tropics and in desert regions with high ground albedo. Meanwhile, the demand for detecting and quantifying greenhouse gas emissions on various scales calls for supplementing the existing ground-based networks with additional spectrometers. The portable spectrometer EM27/SUN operated in the framework of Collaborative Carbon Column Observing Network

(COCCON) has proven its ability of measuring columnar abundances of greenhouse gases with high reliability. The work presented here overlaps with the Fiducial Reference Measurements for Ground-Based Infrared Greenhouse Gas Observations (FRM4GHG) project funded by ESA. Within FRM4GHG, a COCCON spectrometer is operated in Sodankylä (67.37°N, 26.63°E, 188 a.s.l.) together with other prototype spectrometers. In addition, KIT and IRF operated a second COCCON spectrometer in Kiruna (67.84°N, 20.41°E, 419 a.s.l.). This offers the opportunity of deriving trace gas gradients between the two sites, thereby allowing for an evaluation of TROPOMI's ability to quantify gradients on regional scales. We will present first results of the CH<sub>4</sub> comparison between S5P satellite data, ground-based COCCON measurements and Copernicus Atmospheric Monitoring Service (CAMS) reanalysis data at the Kiruna and Sodankylä stations for one year and of the CO<sub>2</sub> comparison between COCCON and CAMS data for a few years. We will assess the ability of the S5P satellite and CAMS of reproducing gradients of GHG fields on regional scales in boreal Scandinavia.

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#### **TROPOMI NO<sub>2</sub> slant column retrieval: comparisons against OMI/QA4ECV**

*Dr Jos Van Geffen<sup>1</sup>, Dr Folkert Boersma<sup>1,2</sup>, Dr Henk Eskes<sup>1</sup>, Dr Maarten Sneep<sup>1</sup>, Mark ter Linden<sup>1,3</sup>, Marina Zara<sup>1,2</sup>, Dr Pepijn Veefkind<sup>1,4</sup>*

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The retrieval of TROPOMI nitrogen dioxide (NO<sub>2</sub>) concentrations is a 3-step procedure: slant column density (SCD) retrieval, separation of the SCD in its stratospheric and tropospheric components, and conversion of these into vertical column densities.

The poster focusses on the comparison of NO<sub>2</sub> SCD retrieval results from TROPOMI against those of OMI results obtained within the QA4ECV project: comparison of the SCDs itself and of the SCD error estimated as well as the statistical uncertainty, based on the spatial variability of the SCDs. The comparisons are performed over a remote Pacific Ocean sector, i.e. away from sources of NO<sub>2</sub>.

The results presented on the poster are part of the following paper:

van Geffen, J., Boersma, K.F., Eskes, H., Sneep, M., ter Linden, M., Zara, M. and Veefkind, J.P.: 2019,

"S5P/TROPOMI NO<sub>2</sub> slant column retrieval: method, stability, uncertainties, and comparisons against OMI", AMT, to be submitted.

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#### **Routine Operations Validation Service for Sentinel-5p TROPOMI Atmospheric Level-2 Data Products**

*Dr.ir. Jean-Christopher Lambert<sup>1</sup>, VDAF / VAL Team of the Sentinel-5p Mission Performance Centre (MPC)*

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This poster overviews the activities and public outcome of the Copernicus Sentinel-5p Routine Operations Validation Service operated in the framework of ESA's Sentinel-5p Mission Performance Centre (S5P MPC). The service has been provided for Level-1 and Level-2 data products generated by both the Near Real Time (NRTI) and Offline (OFFL) processors since the first public data release in July 2018. Routine operations validation activities update, detail and complement the quality information described in the Product Readme Files (PRF) delivered with the S5P data products, in which users can find S5P data usage recommendations. The service produces quarterly a Consolidated Validation Report (ROCVR) integrating results from the MPC operational Validation Data Analysis Facility (VDAF) Automated Validation Server (AVS) and from independent analysis carried out by the MPC VAL consortium, with ad hoc support from S5P Validation Team (S5PVT) AO projects. S5P data quality information is made available publicly through the TROPOMI operational validation website at <http://mpc-vdaf.tropomi.eu>

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#### **Application of Sentinel-5P observations for estimation of nitrogen oxides fluxes from power plants in Poland**

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<sup>3</sup>Institute of Geophysics, Polish Academy of Sciences

The most significant point sources of nitrogen oxides are associated with power plants. The fourth-largest fossil-fuel power station is situated in central Poland near Bełchatów. It is the world's largest lignite-fired power station.

In this study, we calculate column NO<sub>2</sub> from a chemical weather model, GEM-AQ. The model is run operationally at 2.5km resolution over Poland. The vertical domain of the model extends to 10 hPa. Emission inventories are prepared using the bottom-up approach. Characteristics of significant NO<sub>2</sub> point sources were calculated using both model and TROPOMI data. By slicing across wind direction, NO<sub>2</sub> plumes were examined. The diffusion coefficient was estimated based on Gaussian distribution fit with a steady-state assumption.

Lifetime and emission flux on nitrogen oxides were estimated by integrating across wind direction. Differences between GEM-AQ and TROPOMI results were discussed, and significant sources of uncertainty were identified.

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#### **Testing an automated enclosure system for a ground-based shortwave infrared remote sensing spectrometer; application to the validation of Sentinel-5 Precursor carbon monoxide and methane**

*Dr. Neil Humpage<sup>1</sup>, Prof. Hartmut Boesch<sup>1,2</sup>, Mr Florian Dietrich<sup>3</sup>, Prof Jia Chen<sup>3</sup>*

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The Bruker EM27/SUN Fourier transform spectrometer is designed to observe column-average concentrations of the greenhouse gases (GHGs) carbon dioxide and methane, along with other gases including water vapour and carbon monoxide, by measuring high resolution (0.5 cm<sup>-1</sup>) near- to shortwave infrared spectra which use the sun as the light source. These instruments provide frequent observations over a location of interest, complementary to satellite observations (e.g. TROPOMI, OCO-2/3, GOSAT, TANSAT) that give global coverage on a much less frequent basis (once a day in the case of TROPOMI, which flies on board the Copernicus Sentinel-5 Precursor). Since they are portable, EM27/SUNs can be used to fill gaps in ground-based validation networks in regions where the infrastructure isn't in place to support a more permanent deployment (Frey et al 2019). They are also suitable for short term campaigns, where a network of EM27/SUNs are set up to quantify the emissions from an extended GHG source such as a city (Hase et al 2015, Chen et al 2016).

Here we describe the testing of an automated enclosure designed by the Technical University of Munich (Heinle and Chen 2018) for continuous operation of the EM27/SUN in all weather conditions. As well as

weather-proofing the instrument, the enclosure enables remote control of the spectrometer. This allows the EM27/SUN to be deployed in locations where daily supervision of the equipment is impractical, and means that a single person is able to monitor a network of EM27/SUNs across several locations. We show results from testing of the system at the University of Leicester during summer 2019, in preparation for a longer-term deployment in Uganda as part of the NERC MOYA project studying the global methane budget. We pay particular attention to our column-average concentration measurements of carbon monoxide and methane, the two gases retrieved from the Sentinel-5 Precursor TROPOMI shortwave infrared band.

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#### **Sentinel-5P and ground based measurements of methane over Sodankylä, Finland**

*Dr. Rigel Kivi<sup>1</sup>, Pauli Heikkinen<sup>1</sup>, Ella Kivimäki<sup>1</sup>, Pauli Putkiranta<sup>1</sup>, Juha Hatakka<sup>1</sup>, Tuomas Laurila<sup>1</sup>, Hannakaisa Lindqvist<sup>1</sup>, Johanna Tamminen<sup>1</sup>, Iolanda Lalongo<sup>1</sup>, Tomi Karppinen<sup>1</sup>, Otto Lamminpää<sup>1</sup>, Huilin Chen<sup>2</sup>, Mahesh Kumar Sha<sup>3</sup>, Bavo Langerock<sup>3</sup>*

<sup>1</sup>*Finnish Meteorological Institute, <sup>2</sup>Center for Isotope Research, University of Groningen, <sup>3</sup>Royal Belgian Institute for Space Aeronomy*

Methane column observations have been performed at Sodankylä in northern Finland since early 2009, using a Fourier Transform Spectrometer (FTS). The instrument records high-resolution solar spectra in the near-infrared spectral region. From the measured spectra column-averaged abundances of several gases, including methane, are derived. The instrument at Sodankylä participates in the Total Carbon Column Observing Network (TCCON). The TCCON measurements have been widely used for the validation of satellite based observations. Here we report FTS measurements at Sodankylä and comparisons with the TROPOspheric Monitoring Instrument (TROPOMI) on board of the Copernicus Sentinel-5 Precursor satellite, based on the work within HIGHVAL project (High latitudes validation for TROPOMI/S5P). HIGHVAL is focusing on aspects that are typical for high latitudes, including stratospheric vortex conditions, high solar zenith angles and snow-covered surface conditions. Comparisons between TROPOMI and ground based FTS methane measurements show seasonal dependency during years 2018 and 2019. We are investigating the source of the seasonal bias by evaluating the effect of albedo and a priori profiles. Year around AirCore observations have been performed at Sodankylä to validate remote sensing retrievals. Recently we have performed first coordinated balloon and drone borne

AirCore flights. The combination of the drone based and balloon based measurements can be used to reduce uncertainties of the profiles obtained in the lowermost atmospheric layers.

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### **Validation of TROPOMI methane with TCCON: Reduced intercomparison errors by using independent a priori profile information**

*Mr. Johannes Lutzmann<sup>1,2</sup>, PD Dr. Ralf Sussmann<sup>2</sup>, Dr. Thomas Blumenstock<sup>3</sup>, Dr. Tobias Borsdorff<sup>4</sup>, Prof. Dr. Huilin Chen<sup>5</sup>, Dr. Frank Hase<sup>3</sup>, Dr. Rigel Kivi<sup>6</sup>, Prof. Dr. Justus Notholt<sup>7</sup>, Prof. Kimberly Strong<sup>8</sup>, Dr. Aki Tsurata<sup>9</sup>, Dr. Thorsten Warneke<sup>7</sup>*

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Within the ESA project TCCON4S5P (ID 28603) accurate ground reference for methane (CH4) measurements of the Tropospheric Monitoring Instrument (TROPOMI) on-board the ESA satellite Sentinel-5 Precursor (S5P) is provided using ground-based FTIR soundings from the Total Carbon Column Observing Network (TCCON).

When comparing retrievals of two independent remote sensing instruments, large biases can occur, depending on the dynamic situation affecting the vertical concentration profile of the gas species observed. This intercomparison error arises because the a priori information used in the retrievals of the two instruments is both different (instrument 1 vs. instrument 2) and, to some extent, unrealistic (instrument 1/2 vs. reality). Problems typically occur where the real vertical profiles exhibit an extreme variability in shape: E.g. Ostler et al. (2014) found unacceptably large biases in column-averaged CH4 (up to 30 ppb), comparing mid- and near-infrared FTIR (NDACC vs. TCCON) measurements over the Arctic observation site Ny Ålesund during stratospheric subsidence events. Such effects were found to diminish towards lower latitudes, i.e. the intercomparison error produced a significant latitudinal bias. Also seasonal biases turned out to critically depend upon the detailed choice of a priori profile. Obviously, such biases are also expected to occur in the comparison of TROPOMI vs. TCCON, effectively rendering TCCON validation data

from high-latitude sites less suitable for validation purposes.

To overcome this drawback, the goal of this work is to reduce the intercomparison error via the use of independent profile information. This effort is led by KIT/University of Augsburg, and related commitments are fulfilled within the German DLR-funded project S5P-FTIR-UniA. We try to find an optimum reduction of the intercomparison error by correcting the satellite and ground retrievals to a common a priori which resembles the true concentration profile at the moment of observation as closely as possible. Past work like Sussmann et al. (2013) and Ostler et al. (2014) demonstrated the potential of this method to reduce the intercomparison error by applying modelled vertical profiles from a chemistry transport model as common a priori for NDACC and TCCON measurements of CH4. Similarly, in our current work, we compare the use of CarbonTrackerEurope-CH4 (CTE-CH4) data assimilation system (Tsurata et al. 2017) as a source of common a priori information for the validation of the TROPOMI XCH4 with TCCON retrievals with the common use of the original a priori profiles of either measurement system. The accuracy of the respective profiles in representing true atmospheric CH4 concentrations is evaluated for the high-latitude TCCON site of Sodankylä using available AirCore (Karion et al. 2010) in-situ profile measurements, conducted in the framework of the FRM4GHG and RINGO projects in 2017 and 2018. In our poster we will elaborate on the effect of using the named sources for common a priori profiles on the bias between TROPOMI and TCCON XCH4 and show how this effect relates to their accuracy with respect to AirCore profiles.

#### **Acknowledgments:**

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### **Comparison of Sentinel 5 Precursor/TROPOMI NO<sub>2</sub> observations with LOTOS-EUROS simulations and ground-based in situ measurements in Mediterranean cities.**

*Ms. Ioanna Skoulidou<sup>1</sup>, Dr. Maria-Elissavet Koukouli<sup>1</sup>, Dr. Arjo Segers<sup>2</sup>, Dr. Astrid Manders<sup>2</sup>, Dr. Trissevgeni Stavrakou<sup>3</sup>, Prof. Dimitrios Balis<sup>1</sup>, Dr. Jos van Geffen<sup>4</sup>, Dr. Henk Eskes<sup>4</sup>*

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Chemical Transport Models (CTM) and satellite observations are essential tools for studying and estimating NO<sub>2</sub> emissions, concentrations and dynamics in high spatial and temporal resolution. In this study, the regional air quality model LOTOS-EUROS v2.2 is used for the estimation of NO<sub>2</sub> tropospheric columns over Europe with a spatial resolution of 0.25°x0.25° for the year 2018, which then are compared against S5P/TROPOMI daily tropospheric NO<sub>2</sub> data extracted from the TEMIS repository. The CAMS v2.2.1 emission inventory is ingested into LOTOS-EUROS for the simulation, while the initial and boundary conditions are retrieved from the CAMS Near-real-time dataset. Finally, LOTOS-

EUROS is fed with meteorological data from the operational dataset of ECMWF. Higher spatial resolution runs (0.1°x0.1°) are then conducted for smaller regions around the Mediterranean and compared with the S5P/TROPOMI tropospheric NO<sub>2</sub> columns, after applying the TROPOMI averaging kernels to the modelled results. In this case, the simulations from the LOTOS-EUROS run of the larger region are used as initial and boundary conditions. We further present first comparisons of the modelled NO<sub>2</sub> concentrations with ground-based in situ measurements.

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### **Synergistic use of meteorological imager for aerosol retrieval algorithm of hyperspectral UV-Vis instrument**

*Sujung Go<sup>1</sup>, Professor Jhoon Kim<sup>1</sup>, Professor Sangseon Park<sup>2</sup>, Graduate Student Hyunkwang Lim<sup>1</sup>*

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Successful launch of the Tropospheric Monitoring Instrument (TROPOMI) onboard the Copernicus Sentinel-5 Precursor satellite opens up a new possibility to provide UV aerosol absorption information with higher spatial resolution. However, still the aerosol products retrieved from TROPOMI instrument may have aerosol type selection problem and cloud contamination issue including cirrus cloud contamination.

In this study, aerosol retrieval algorithm with synergistic use of broadband meteorological imager are investigated. Aerosol products, such as aerosol optical depth, single scattering albedo, and aerosol layer height, are retrieved with Level 1B data of Ozone Monitoring Instrument (OMI) using aerosol algorithm prepared for Geostationary Environmental Monitoring Spectrometer (GEMS). For synergistic use of meteorological imager, Moderate Resolution Imaging Spectroradiometer (MODIS) instruments are used. First, synergistic use of cloud masking from meteorological imager infrared (IR) channel was tested. IR channels of meteorological imager help mask cirrus clouds for GEMS aerosol retrieval results. Second, Total Dust Confidence Index (TDCI) was developed for IR channels of meteorological imager to separate dust aerosols, and then applied to improve GEMS aerosol type algorithm. Statistical analysis showed that accuracy for dust aerosols of GEMS are changed from 72% to 94% by using TDCI for aerosol type selection. Third, corrected aerosol types were applied to GEMS algorithm. After applying TDCI as a dust type detection of GEMS aerosol algorithm, the retrieved results of SSA were improved especially for BC and DS aerosols. These improved results are consistent with GEMS aerosol

algorithm sensitivity test about aerosol type misclassification. Finally, AOD products from GEMS and meteorological imager were combined using the maximum likelihood estimate (MLE) method using weights derived from the root mean square error (RMSE) of the original AOD products. Due to the advantage of allowing retrieving aerosol over bright surfaces from the UV-Vis channel, the combined AOD products showed increasing spatial coverage compared to the any of the original products. Moreover, the accuracy was comparable to the any of the original AOD products. Synergistic use of meteorological imager implies the future capability of improving TROPOMI aerosol products using meteorological instruments.

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### The 2018 fire season in North America as seen by TROPOMI:aerosol layer height validation and evaluation of model-derived plume heights

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Before the launch of TROPOMI, only two other satellite instruments were able to observe aerosol plume heights

globally, MISR and CALIOP. The TROPOMI aerosol layer height is a potential game changer, since it has daily global coverage and the aerosol layer height retrieval is available in near-real time. The aerosol layer height can be useful for aviation and air quality alerts, as well as for improving air quality forecasting related to wildfires. Here, TROPOMI's aerosol layer height product is evaluated with MISR and CALIOP observations for wildfire plumes in North America for the 2018 fire season (June to August). Further, observing system simulation experiments were performed to understand the fundamental differences between the different products. The results show that MISR and TROPOMI are, in theory, very close for aerosol profiles with single plumes. For more complex profiles with multiple plumes, however, different plume heights are retrieved: the MISR

plume height represents the top layer, and the plume height retrieved with TROPOMI tends to be an average altitude of several plume layers.

The comparison between TROPOMI and MISR plume heights shows, that on average, the TROPOMI aerosol layer heights are lower, by approximately 600 m, compared to MISR which is likely due to the different measurement techniques. From the comparison to

CALIOP, our results show that the TROPOMI aerosol layer height is more accurate for thicker plumes and plumes below approximately 4.5 km.

MISR and TROPOMI are further used to evaluate the plume height of Environment and Climate Change Canada's operational forecasting system FireWork with fire plume height estimates from the Canadian Forest Fire Emissions Prediction System (CFFEPS). The modeled plume heights are similar compared to the satellite observations, but tend to be slightly higher with average differences of 60-320m and 270-580m compared to TROPOMI and MISR, respectively.

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### German campaign activities for the uncertainty characterization of trace gas products from Sentinel-5p

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The Sentinel-5-precursor (S5p) satellite with the TROPOMI payload was launched on 13 October 2017. It is part of the Copernicus programme and provides products of atmospheric constituents related to air quality and climate change with almost daily global coverage. The good quality of the instrument enables precise measurements despite the fine spatial resolution of 3.5 x 5.5 km<sup>2</sup>. The accuracy is impacted by the uncertainties from auxiliary datasets required in the retrieval of Level2 trace gas products, such as information on clouds, aerosols, surface reflectance and the trace gas profile.

In order to assess the uncertainties of the S5p trace gas products a set of different dedicated field studies are planned in the period 2019 – 2020 in the frame of the ESA funded QA4EO Atmospheric Composition Uncertainty Field Studies project taking place in Belgium, the Netherlands, Romania, France and Germany.

Here, we present the activities of the German field study carried out in October 2019. The German activities are focussing on the Ruhr area which is a pollution hotspot in Europe. The campaign

instrumentation consists of airborne, mobile-car and stationary ground-based components.

The airborne component comprises the airborne imaging instrument “AirMAP” developed at IUP Bremen, as well as a small nadir-only Avantes-based instrument, both installed on the FUB Cessna.

Three mobile DOAS instruments are installed on cars that are deployed in the area covered by the flights. These instruments are operated by IUP-Bremen, BIRA-IASB and MPIC (together with AIOFM).

Stationary instruments are installed in or close to the target areas for a longer period than the actual time frame of the mobile deployments. These measurements will help to interpret the mobile campaign dataset and can also be used for S5p uncertainty estimation themselves. This stationary component comprises three Pandora instruments operated by NASA and FU Berlin, three zenith-sky DOAS instruments operated by IUP-Bremen and a MAX-DOAS instrument operated by BIRA-IASB. In addition we make use of routinely operated infrastructure, such as an AERONET station and the in-situ air quality network.

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